Plenary Lecture : **PLEN-1**

Plenary Lecture

Multipurpose Hall 1 THU 13:30

Chair: Chulbom Lee (Seoul National University)

Catalytic C-H Amination Reactions: Scope and Intermediacy of Metal Nitrenoids

Sukbok Chang

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

Direct amination of C–H bonds is a highly desirable reaction due to the significant utility of aminated products in total synthesis, medicinal chemistry and materials science. Despite substantial research efforts, particularly in recent years, the current status of achieving C–H amination reactions with high stereoselectivity and turnover numbers remains still limited. In this context, we have developed a series of novel methodologies that employ tailor-made transition metal catalysts in combination with dioxazolones as robust nitrenoid precursors. We explored applicable substrates, including a wide range of readily available compounds such carboxylic acids and hydrocarbons, for both intra- and intermolecular amination reactions. By optimizing the individual chiral catalyst system, we subsequently developed asymmetric transformations, achieving an excellent level of enantioselectivity to produce chiral azacyclic compounds (β-, γ-, and δ-lactams). Furthermore, we successfully validated, for the first time, the intermediacy of the presumed but highly elusive metal acylnitrenoid through a photocrystallographic approach, thus addressing long-standing challenges in this field.

Award Lecture : **AWARD-1**

Award Lecture - 2023 Taikyue Ree Academic Award

Multipurpose Hall 1 FRI 13:30

Chair: Zee Hwan Kim (Seoul National University)

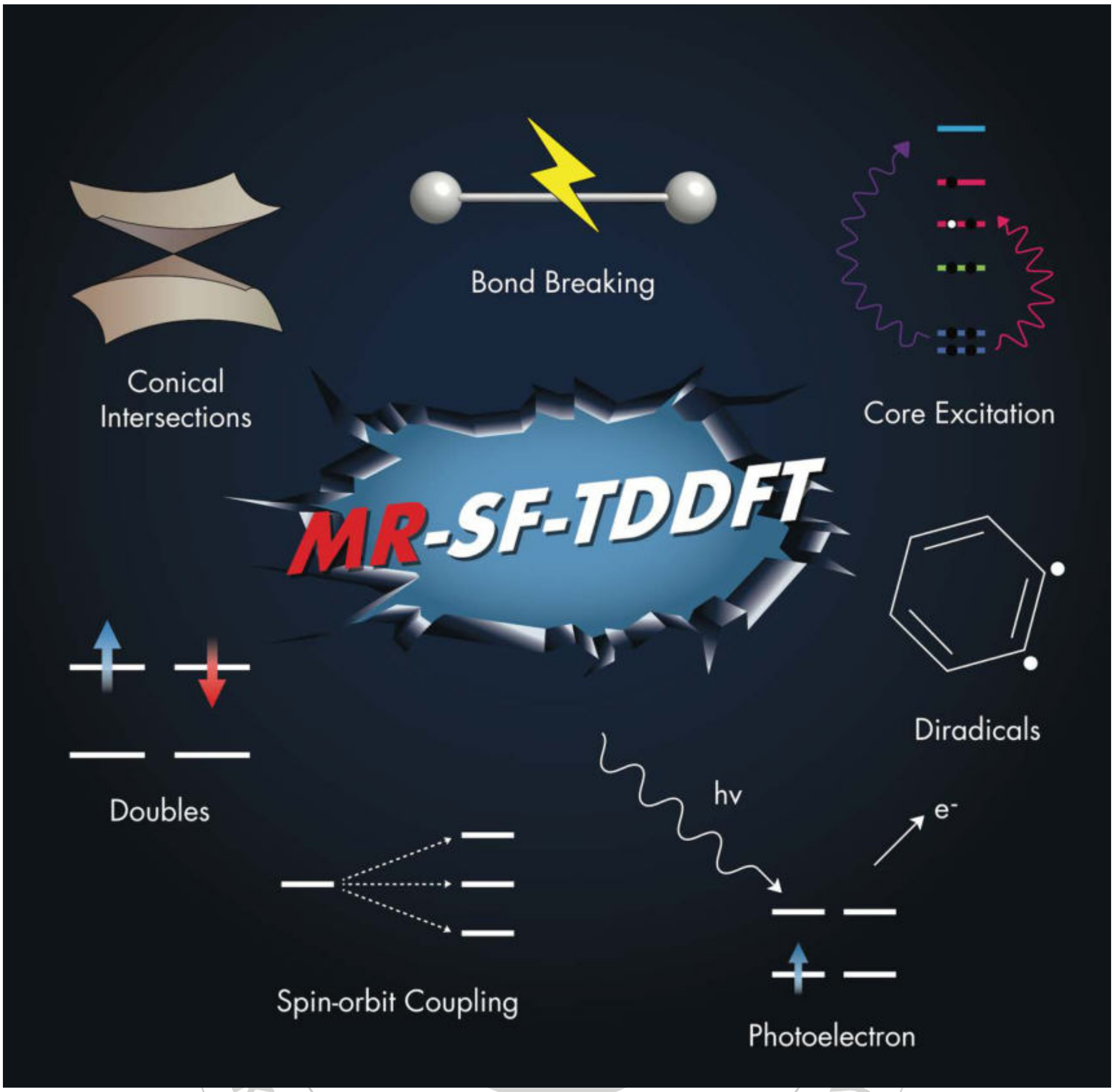
MR-SF-TDDFT: A Breakthrough in the Study of Strongly Correlated Systems

Cheol Ho Choi

Department of Chemistry, Kyungpook National University, Korea

A new quantum theory, MRSF-TDDFT (Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory) has been developed*, which introduces the multi-reference advantages within the linear response formalism. The density functional theory (DFT) and linear response (LR) time-dependent (TD)-DFT are of utmost importance for routine computations. However, the single reference formulation of DFT is suffering from the description of open-shell singlet systems such as diradicals and bond-breaking. LR-TDDFT, on the other hand, finds difficulties in the modeling of conical intersections, doubly excited states, and core-level excitations. Many of these limitations can be overcome by MRSF-TDDFT, providing an alternative yet accurate route for such challenging situations. Empowered by the practicality of LR formalism, it is anticipated that MRSF-TDDFT can become one of the major workhorses in general routine tasks. Now the theory is combined with NAMD, QM/MM, Spin-Orbit Couplings, and Extended Koopman Theorem. Here, we highlight its performances by presenting our recent results by MRSF-TDDFT especially focusing on nonadiabatic molecular dynamics.

(a) Lee, S., Filatov, M., Lee, S., & Choi, C. H. (2018). J. Chem. Phys., 149(10), 104101.
(b) Lee, S., Kim, E., Nakata, H., Lee, S. & Choi, C. H. (2019). J Chem. Phys., 150(18), 184111.


Conical Intersections
Bond Breaking
Core Excitation
MR-SF-TDDFT
Diradicals
Doubles
hν
e⁻
Spin-orbit Coupling
Photoelectron

Symposium : **KCS1-1**

[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry

Room 201+202+203 WED 13:10

Chair: Mi Hee Lim (KAIST)

Crafting Designer Nanoreactors for Bio-orthogonal Catalysis in Living Systems

In Su Lee

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

Bio-orthogonal catalysis offer a highly versatile toolkit for biochemical modulation and capability to perform new-to-nature reactions inside living systems, endowing advanced biotechnologies. However, conventional catalysts have limitations to control the reactions under physiological conditions. In our research over past years, our aim has been to bridge the advanced field of molecular synthesis with broader areas of biological and biomedical science by developing multicomponent designer nanoreactors (NRs) where surface-composition, morphologies, interfacial active-sites and microenvironment around different metal nanocatalysts can be precisely controlled by novel nanospace-confined chemistries. For example, we have designed and synthesized different plasmonically integrated NRs with plasmonic-catalytic compartments, hollow bilayer nanospace and metal-laminated nanocrystal inside hollow silica to perform NIR/light-induced catalytic reactions in complex media including living cells. We also demonstrated magnetothermia-induced NR, carrying a preinstalled superparamagnetic iron-oxide core inside a hollow-porous silica nanoshell, to endow the opportunity to apply magnetic field as biorthogonal stimulus to promote catalytic reactions. In this talk, I will share those recent results and discuss our research direction to promote organic reactions in complex bio-media and living cells by using designer NRs.

Symposium : **KCS1-2**
[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry
Room 201+202+203 WED 13:30
Chair: Mi Hee Lim (KAIST)

Bioinorganic Strategies to Understand Multiple Facets in Neurodegenerative Disorders

Mi Hee Lim

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

Neurodegeneration associated with Alzheimer's disease (AD) is related to multiple interconnected features, including (i) the accumulation of amyloid-β (Aβ) aggregates, (ii) metal ion misregulation, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). Recent efforts have made to determine the inter-relations between some of these pathological factors. Metals are found entangled in Aβ plaques and likely contribute to Aβ-induced toxicity and oxidative stress. ROS have been shown to increase the rate of Aβ plaque formation. Our understanding of the correlation between these elements and AD pathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.[1-3] To advance our understanding of AD pathogenesis and find an effective cure for AD, the relationship between various causative factors of this devastating disease should be addressed. Towards this goal, we have been developing chemical tools or strategies capable of modulating multiple underlying factors or identifying the pathogenic networks composed of their direct interactions and reactivities.[4-11]References(1)*Chem. Soc. Rev.* 2012, *41*, 608.(2)*Acc. Chem. Res.* 2014, *47*, 2475; Acc. Chem. Res. 2021, *54*, 3930.(3)*Chem. Rev.* 2019, *119*, 1221.(4) *Proc. Natl. Acad. Sci. USA* 2010, *107*, 21990.(5) *Chem. Sci.* 2015, *6*, 1879.(6) *J. Am. Chem. Soc.* 2014, *136*, 299.(7) *J. Am. Chem. Soc.* 2015, *137*, 14785.(8) *Nat. Commun.* 2016, *7*, 13115.(9)*Proc. Natl. Acad. Sci. USA* 2020, *117*, 5160.(10) *J. Am. Chem. Soc.* 2020, *142*, 8183.(11) *Nat. Chem.* 2022, *14*, 1021-1030.

Symposium : **KCS1-3**
[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry
Room 201+202+203 WED 13:50
Chair: Mi Hee Lim (KAIST)

A photo-responsive iron-nitrosyl complex in acute vascular occlusion disease

Jaeheung Cho

Department of Chemistry, UNIST, Korea

The development of metallodrugs, a class of therapeutic agents containing metal ions, has emerged as a crucial avenue in modern medicinal chemistry. Their unique properties and interactions offer distinct advantages, revolutionizing the landscape of drug design, and opening new possibilities for targeted treatments and enhanced therapeutic efficacy.Retinal vascular occlusion is a prevalent cause of visual impairment. While various approaches, including vasodilators, have been investigated for the treatment, there is currently no effective method available. Herein, we present a novel strategy for treating vascular occlusions by using a photo-responsive iron-nitrosyl complex, [Fe(TBDAP)(NO)(H2O)]2+ (1), which acts as a spatiotemporally controllable nitric oxide transporter. Complex 1 was synthesized and characterized using various chemicophysical techniques including X-ray crystallography. Its ability to selectively dilate normal retinal blood vessels and reperfuse the occluded vessels was demonstrated in animal disease models.

Symposium : **KCS1-4**
[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry
Room 201+202+203 WED 14:30
Chair: Inji Shin (Seoul National University of Science and Technology)

Lessons from COVID-19 for the development of antiviral drugs

Soo bong Han

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

The global response to the COVID-19 pandemic has yielded significant insights that can guide the future development of antiviral drugs. It is important to address the valuable insights gained from the pandemic, which can be utilized to improve the efficiency and effectiveness of strategies for developing antiviral drugs. The urgency of the pandemic underscored the importance of expediting drug development without compromising safety, leveraging innovative technologies and collaborative approaches. Global cooperation and data sharing were paramount, highlighting the need for open communication and resource pooling. The value of broad-spectrum antiviral activity was underscored, offering a versatile approach to combatting multiple viral threats. Repurposing existing drugs for new indications proved successful, demonstrating the potential for accelerated responses. Given the rapid mutation rates of viruses, designing drugs to target critical points in viral replication cycles and considering adaptable drug designs are critical. Combination therapies emerged as a robust strategy, minimizing drug resistance and enhancing efficacy. Clinical trial readiness, sustained research investment, and equitable manufacturing and distribution strategies are essential to streamline drug development and ensure timely global access. In conclusion, the lessons derived from the COVID-19 pandemic offer a roadmap for optimizing antiviral drug development processes, ultimately bolstering global preparedness against future viral outbreaks.

Symposium : **KCS1-5**

[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry

Room 201+202+203 WED 14:50

Chair: Inji Shin (Seoul National University of Science and Technology)

Discovery of potent and selective Keap1/Nrf2 modulators for the treatment of Alzheimer’s disease

Ki Duk Park

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

Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by deposition of neuropathological aggregates such as amyloid-β and neurofibrillary tangle and subsequent cognitive impairment. In the early stages of AD, oxidative stress and neuroinflammation due to excessive glial activation have been reported to exacerbate pathology and progression of AD. The kelch-like ECH-associated protein 1 (Keap1)-nuclear factor E2-related factor 2 (Nrf2) signaling pathway is a major antioxidant defense system and is also involved in anti-inflammatory responses. Here, we show that pharmacological activation of Nrf2 through selective modification of cysteine 151 in Keap1 has potent antioxidant and anti-inflammatory effects in murine glial cells. Administration of Nrf2 activator reversed cognitive decline and prevented AD-like pathologies including glial hyperactivation, neuroinflammation, and Aβ deposition in APP/PS1 mice. Additionally, we identified the regulatory mechanisms of Keap1-Nrf2 signaling in terms of disease-associated astrocytes and microglia in AD. These findings suggest that Keap1-Nrf2 signaling could be assessed as an emerging therapeutic target for prevention and treatment of AD.

Symposium : **KCS1-6**

[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry

Room 201+202+203 WED 15:10

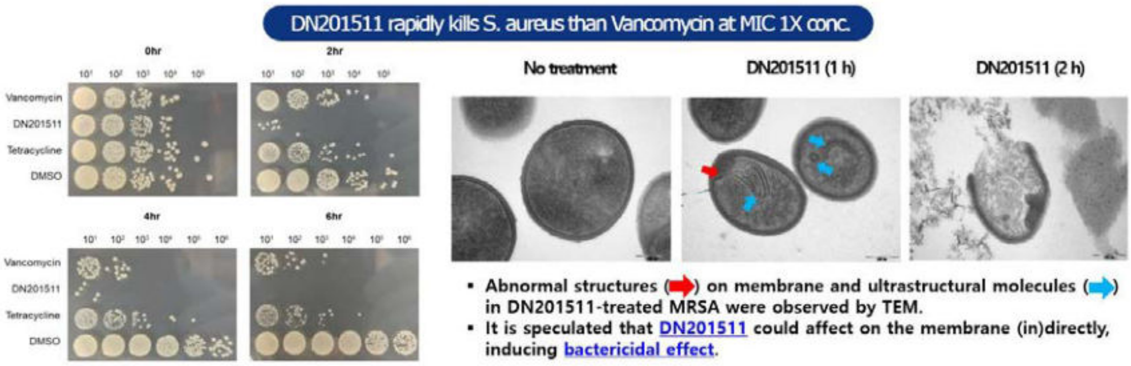
Chair: Inji Shin (Seoul National University of Science and Technology)

Development of Prokaryotic UMP Kinase (pyrH) Inhibitor Towards the Novel Class of Broad-Spectrum Antibiotics

Soong-Hyun Kim

New Drug Development Center, K-MEDI hub, Korea

Due to overusing antibiotics, antimicrobial resistance has been serious problem in public health. Methicillin resistant Staphylococcus aureus (MRSA) is one of the multi-drug resistant bacteria and a main cause of several difficult-to-treat infections in humans. For the effective treatment of the antibiotic resistances, a novel class of antibiotics is required to develop. We have screened the in-house compound-library, not open-sources of compound-libraries, to check antibacterial activities against MRSA. DN201511 was the compound with MIC50 ~5 uM against the various MRSA strains. Interestingly, DN201511 demonstrates the bactericidal activity, faster than Vancomycin, constructing abnormal molecules inside MRSA. The transcriptomic analysis of DN201511 treated MRSA culminated in the identification of a novel target of UMP kinase (pyrH) in the pyrimidine biosynthesis pathway. DN201511 inhibits pyrH (IC50 ~5 uM), which was recombinant protein of Staphylococcus aureus. Moreover, DN201511 shows the submicromolar activities against Vancomycin resistant Enterococci (VRE). DN201511 also shows the remarkable synergistic effect by combi-therapy with collistin against Pseudomonas aeruginosa (PAO1, Gram negative bacteria). Currently, more than 140 compounds were synthesized for the lead optimization, directed towards the development of broad-spectrum antibiotics. The crystal study of the inhibitor bound to pyrH is on-going for the structure-based drug discovery as well. Detailed biological data, SAR analysis, and efficacy data in the table of target product profile are presented in this talk.



DN201511 rapidly kills S. aureus than Vancomycin at MIC 1X conc.

- Abnormal structures (➡) on membrane and ultrastructural molecules (➡) in DN201511-treated MRSA were observed by TEM.
- It is speculated that DN201511 could affect on the membrane (in)directly, inducing bactericidal effect.

Symposium : **KCS1-7**
[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry
Room 201+202+203 WED 15:50
Chair: Sun-Joon Min (Hanyang University)

Cytochrome c-based systems for artificial photosynthesis

Kara L. Bren

Department of Chemistry, University of Rochester, United States

The storage of solar energy in the form of chemical fuels is an approach to expanding our use of the sun as a renewable and clean energy resource. Such systems require light absorption, charge separation, and catalysis of energy storing reactions. In this work, we are constructing systems for artificial photosynthesis that utilize cytochromes as components for catalysis and charge transfer. For catalysis of fuel production from abundant feedstocks, semisynthetic and synthetic cytochromes are developed for proton reduction to dihydrogen and carbon dioxide reduction to carbon monoxide. To build systems for light driven fuel production, these catalysts are paired with molecular or nanocrystalline photosensitizers. The initial systems developed use sacrificial electron donors. In a more sustainable approach, we report the use of engineered bio-nano systems which respiratory electrons from the bacterium Shewanella oneidensis provided via cell-surface cytochromes c sustain photochemical hydrogen production in living bio-nano systems. These bio-nano systems produce hydrogen for weeks provided lactate is present as a nutrient. Ongoing work includes the investigation of the mechanism of charge transfer from bacteria to nanoparticles, optimization of which is expected to yield more highly active systems.

Symposium : **KCS1-8**
[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry
Room 201+202+203 WED 16:30
Chair: Sun-Joon Min (Hanyang University)

Metal Nitrosyls That Mimic Global Nitrogen Cycle Transformations: Generation of Reduced NO_x Species

Todd C. Harrop

Department of Chemistry and Center for Metalloenzyme Studies, The University of Georgia, United States

Nitrogen is an essential element for all forms of life on this planet. As such, nature has evolved metalloenzymes to utilize the N_2 present in the atmosphere and convert it to more bioavailable forms such as ammonia. This process and the chemical reactions transforming inorganic N-containing small molecules in general, is part of the Global Nitrogen Cycle (GNC). The GNC describes the conversions of all environmentally-relevant N-containing species on this planet including nitrate (NO_3–), nitrite (NO_2–), nitric oxide (NO), nitrous oxide (N_2O), etc. where Fe-containing enzymes play a central role. Attention in the chemical transformations of select nitrogen oxides (NO_x) has heightened due to the overuse of nitrogen-rich fertilizers, which has increased the concentration of NO_3– and NO_2– to toxic levels in water runoff. Additionally, other work emphasizes the role of NO_2– as a reservoir of NO for mammals under hypoxic conditions. Indeed, NO_x compounds participate in a wide range of biological processes. Of interest to our group is the metal-promoted reduction of NO_2– to produce NO (and eventually NH_3) as well as the construction of metal-bound nitroxyl (NO– or HNO) coordination complexes. This seminar describes our efforts in understanding the fundamental bioinorganic chemistry of NOx reduction mediated by non-porphyrin Fe and Co systems.

Symposium : **KCS1-9**

[Chemistry Symposium for Future Innovation & BKCS Symposium] The Story of Our Lives Fashioned by Chemistry

Room 201+202+203 WED 17:10

Chair: Sun-Joon Min (Hanyang University)

Catalytic Oxidation of C-H Bonds with O_2 in aqueous solvents

Abhishek Dey

School of Chemical Science, IACS, India

Oxidation of C-H bonds with selectivity and facile rates, but most importantly using O_2, has been a long time goal of chemistry community. Over the last few years, this group has reported creation of mimics of heme dioxygenase, heme monooxygenase and heme peroxidase on self-assembled monolayers of thiols on Au and Ag surfaces. These synthetic bio-inspired systems generate strong oxidants using molecular O_2 which can easily oxidize C-H bonds having BDE>100 Kcal/mol. Mechanistic investigations using in-situ resonance Raman spectroscopy reveal the reactive intermediates (Fe^{III}-O_2- or Fe^{III}-OOH or Fe^{IV}=O or Fe^{V}=O) involved and different oxidants are generated from O_2 at different applied potentials. Using this advantage catalytic dioxygenase type activity and oxidation of toluene to benzaldehyde with TON more than 60000 as well as monooxygenase activity with alkane to alcohol and alkene to epoxide with TON more than 20000 could be attained from the same system by switching the applied potential.

Symposium : **KCS2-1**

[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution

Room 206+207 WED 14:30

Chair: Hyuck Jin Lee (Kongju National University)

A multi-disciplinary approach to the elucidation of protein activities

Seung Jae Lee

Department of Chemistry, Jeonbuk National University, Korea

Proteins have specific structures and functions for biological activities; therefore, active sites have received attention to elucidate their mechanisms. One third of enzymes are considered metalloproteins, which have one or more metal ions and are coordinated for structural and functional roles. In this presentation, soluble methane monooxygenase (sMMO) will be discussed to explain how the activity of sMMO is elucidated through multidisciplinary assays including X-ray crystallography, NMR and cryo-EM methods. sMMO, a bacterial multicomponent monooxygenase superfamily, requires hydroxylase (MMOH), reductase (MMOR), and a regulatory component (MMOB) for its catalytic activities. Recent studies have shown that other auxiliary components are required for sMMO activities, and these enzymatic reactions are monitored by *Methylosinus sporium 5*, a type II methanotroph. The first complex of MMOH-MMOB provides crucial information to understand the binding site of MMOH and substrate pathways to diiron active sites. This is regulated by the modification of long α-helices of MMOH α-subunit, and structural studies have proved that MMOD, an inhibitory component, shares a binding site with MMOB. The other auxiliary enzyme, MMOR, transfers electrons from NADH to diiron active sites through FAD-binding domain and ferredoxin domain. This electron transfer mechanism can be explained by electron paramagnetic resonance (EPR) studies by annealing methods to extract $[2Fe\text{-}2S]^+$ and FAD at 20 and 60 K, respectively. These mechanism studies were further investigated with the help of cryo-EM, which can demonstrate the dynamics of protein-protein interactions in sMMO complexes.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **KCS2-2**
[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution
Room 206+207 WED 14:55
Chair: Hyuck Jin Lee (Kongju National University)

The Contribution of Magnetic Resonance Spectroscopy for Future Innovation

Sun Hee Kim

Western Seoul Center, Korea Basic Science Institute, Korea

As we stand in the middle of the era of the 4th industrial revolution, scientists continue to contribute to develop human knowledge for making the better society. Chemists are not exceptions. As one of chemists, our group focuses on advancing our knowledge for the application of magnetic resonance spectroscopy, in particular electron spin version, EPR spectroscopy to add our efforts to participate this agenda.Along this line, I will introduce the main research topics of our group for the advancement of chemistry education in my talk. The themes of our research can be classified into three topics: 1) Mechanistic studies on bio-mimetic catalytic reaction for energy conversion, 2) Metal ion effect on amyloid peptide fibrilization, 3) Utilizing molecular electronic spin-based qubits for quantum information processing.In this talk, I will present the recent representative results from our group related with these topics together with the recent development of EPR spectroscopy in our group.We hope to continue to play a part in making the better society in the new era of the 4th industrial revolution as chemists.

Symposium : **KCS2-3**
[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution
Room 206+207 WED 15:20
Chair: Hyuck Jin Lee (Kongju National University)

Lessons from Nature and Electronic Structures: Light and O_2 Utilization for Organonickel Chemistry

Kiyoung Park

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

Organonickel complexes are the key intermediates of Ni-catalyzed cross-coupling reactions that can generate various bonds such as C-C, C-N, C-O, and C-S bonds. We have used diverse transition-metal based spectroscopic techniques, such as magnetic circular dichroism, electron paramagnetic resonance, resonance Raman, and X-ray absorption spectroscopies, in combination with density functional theory computations, to characterize the electronic and geometric structures of organonickel (II, III, and IV) complexes. The analyses have revealed that C-based ligands can form more covalent bonds to the nickel center than N- or O-based inorganic ligands and that the level of covalency determines their reductive elimination (RE) activity as well as reductive O_2 activation reactivity. By utilizing structure/function correlations, we have developed excited-state RE reactions without relying on exogenous photosensitizers and O_2-derived oxygenation reactions. The spectroscopic and computational elucidations of reaction intermediates have unveiled that the oxygenation of organonickel complexes can follow the reaction coordinates of non-heme Fe oxygenase enzymes. This finding provides a crucial clue on how to facilitate a rather limited O_2 reactivity in organometallic chemistry, demonstrating the significance of electronic-structure level understanding for systematic design to utilize O_2 not only as an electron acceptor but also as an oxygen atom donor.

Symposium : **KCS2-4**
[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution
Room 206+207 WED 15:55
Chair: Hyuck Jin Lee (Kongju National University)

Vitamins as Potent Anticancer Agents Targeting Matrix Metalloproteinase-2/9

Hyuck Jin Lee

Department of Chemistry Education, Kongju National University, Korea

Over the past few decades, various studies have tried to find better strategies for the treatment of intractable diseases such as cancer. One potential target is Matrix metalloproteinases (MMPs), of which MMP-2 and MMP-9 play a crucial role in the onset and progression of cancer through multiple ways, including tumor cell invasion, angiogenesis, immune evasion, and metastasis. Therefore, several chemical agents have been developed to regulate the expression and activity of MMP-2/9 for treating cancer. Due to the dose limiting toxicity and biosafety, however, the chemicals need to be improved their biological properties. To reduce the risk of toxicity, we explored natural molecules, such as vitamins, as MMP-2/9 regulators. The abnormal amount of vitamins in the body have been linked to various diseases including multiple cancers; prostate, breast, brain, lung, and skin cancer. Therefore, we investigated the relationship between MMP-2/9 and vitamins to better understanding of the pathogenic mechanisms of cancers. In our study, we examined the effect of both fat- and water-soluble vitamins (vitamin A, B6, C, and D3) on the expression and activity of MMP-2/9 through biological and biochemical experiments, and identified the interactions between vitamins and MMP-2/9 through docking simulations. As a result, vitamin A significantly inhibited the activity and expression of MMP-2, while vitamin B6 reduced the levels and actions of MMP-9. Vitamin C and D3 slightly decreased the activity of MMP-2/9. This study could provide new insights into the regulation of MMP-2/9 by vitamins and contribute to the development of a new library for cancer therapy.

Symposium : **KCS2-5**
[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution
Room 206+207 WED 16:20
Chair: Hyuck Jin Lee (Kongju National University)

Recent trends in nanoporous crystalline materials, metal-organic frameworks.

Jin Yeong Kim

Department of Chemistry Education, Seoul National University, Korea

In the rapidly evolving environment of the Fourth Industrial Revolution, the chemistry sector has witnessed profound changes due to the convergence of technology, innovation and interdisciplinary collaboration. As education adapts to prepare students for this new era, there is a pressing need to introduce modern, cutting-edge subjects that resonate with the spirit of the revolution. One such topic with enormous potential is the exploration of metal-organic frameworks (MOFs), a class of porous materials with remarkable structural and functional versatility. MOFs have emerged as noteworthy new materials in modern chemical research due to their unique spatial properties resulting from the combination of metal nodes and organic linkers in well-defined crystal structures. Its high surface area, tunable pore size, and tailor-made chemistry have been well-studied for applications in fields to solve various problems facing humanity, such as gas storage, catalysis, drug delivery, and sensing technologies. This historical development process of MOF can help students solve various problems that society is facing by using MOF, a new chemical material, and stimulate their imagination. By embracing MOF as an educational focus, educators are expected to bridge the gap between traditional chemistry education and the rapidly evolving Fourth Industrial Revolution environment. The inclusion of MOF in chemistry education is expected to serve as a beacon guiding the way to nurture agile and forward-looking chemists.

Symposium : **KCS2-6**
[Chemistry Symposium for Future Innovation] Introduction of Recent Chemistry for the Advancement of Chemistry Education in the New Era of the 4th Industrial Revolution
Room 206+207 WED 16:45
Chair: Hyuck Jin Lee (Kongju National University)

Research trends and directions in chemistry education in the era of the 4th Industrial Revolution

Hyun Kyung Kim[*], **Dong-Heon Lee**[1,*]

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

In the era of the fourth industrial revolution, when society becomes super-intelligent and hyper-connected by digital technology and artificial intelligence, it is difficult to secure individual competitiveness simply by building a lot of knowledge in one field, Instead, integration and convergence between academic fields are emphasized. Furthermore the need for online classes and inquiry activities using information devices such as PCs and smart devices is increasing since the outbreak of COVID-19 pandemic. In response to this need, lots of research are being actively conducted for future convergence education on how students can be equipped with digital knowledge and capabilities in advanced technologies such as AI and SW and have problem-solving skills. We would like to present the results of future convergence education (STEAM) research we are conducting. We present findings of our study on the development and effectiveness of class programs using realistic content such as AR (Augmented Reality) and VR (Virtual Reality) that operate on smart devices. In addition will be presented, class programs using realistic content such as AR and VR in smart devices were developed, and online science virtual experimental contents were developed in a non-face-to-face exploration environment. Development of online science virtual experimental content that can be used and effective in non-face-to-face classes will also be discussed. Through these latest studies, the direction of change in the chemistry curriculum and teaching and learning methods can be explored in preparation for the future society.

Symposium : **KCS3-1**

[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry

Room 208+209+210 WED 13:10

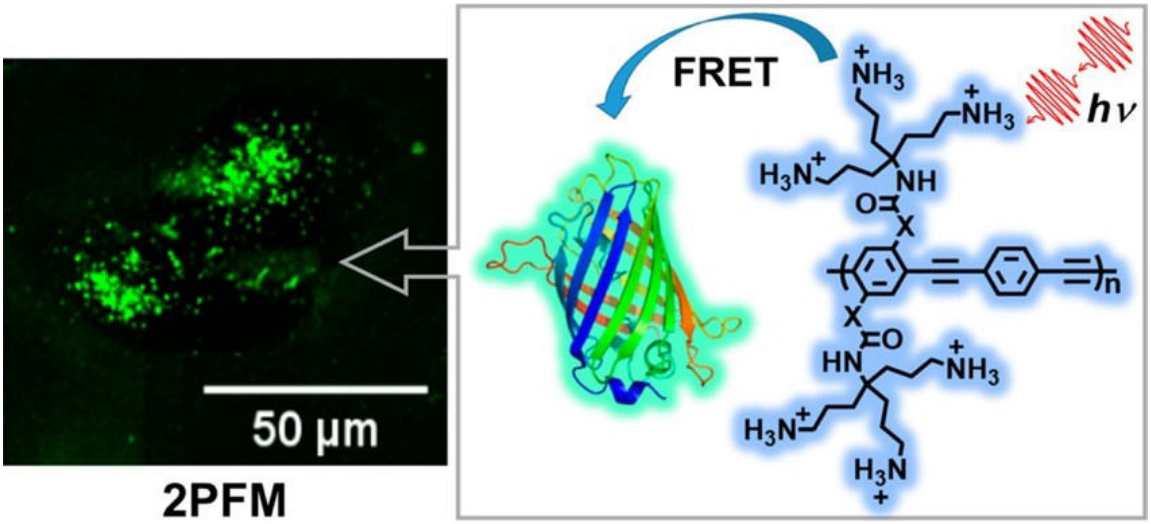
Chair: Songyi Lee (Pukyung National University)

Conjugated Polyelectrolytes in Biosensing and Disinfection

Kirk S. Schanze

University of Texas at San Antonio, United States

Conjugated polyelectrolytes (CPEs) featuring poly(phenylene ethynylene) and poly(thiophene) backbones substituted with ionic solubilizing groups are water soluble. These materials display a variety of interesting properties, including self-assembly into nanoscale aggregates, ability to process into nanostructured layer-by-layer films and optical/stimuli responsive behaviour in the presence of ions, surfactants and biomacromolecules. We have explored the use of cationic CPEs as fluorescent sensors for polyphosphates (pyrophosphate, ATP and ADP). In addition, cationic CPEs exhibit profound light-activated biocidal activity vs. a broad spectrum of bioagents, including bacteria, virus particles and spores. The talk will give a high-level overview work in this area, including recent work concerning the interactions between cationic CPEs and mammalian cells.


50 μm
2PFM
FRET
hν
NH3+
H3N+
NH
O
X
HN
n

Symposium : **KCS3-2**

[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry

Room 208+209+210 WED 13:40

Chair: Songyi Lee (Pukyung National University)

Challenges of treating Alzheimer’s disease

Shikha Nangia

Department of Biomedical and Chemical Engineering, Syracuse University, United States

Finding pathways across biological barriers for delivering life-saving drugs is entering a new era with the rapid advancement of computational resources. My research group focuses on developing simulation methods to elucidate the interfacial phenomenon associated with biological barriers that play a role in life-threatening diseases such as Alzheimer’s, cancer, and chronic infections. Our goal is to influence this experimentally dominated research field by providing mechanistic, structural, and molecular insights into the barrier functions that were computationally unattainable before our work. In the past few years, we have made breakthroughs in understanding the molecular architecture of the blood-brain barrier and developed strategies to enhance the barrier’s permeability for the treatment of neurodegenerative disease. In my talk, I will elaborate on the computational methods we have developed to investigate the blood-brain barrier and provide a perspective on the treatment of Alzheimer’s disease.

Symposium : **KCS3-3**
[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry
Room 208+209+210 WED 14:05
Chair: Songyi Lee (Pukyung National University)

Recent Progress on Phototherapy and Photochemistry

Juyoung Yoon

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Photodynamic therapy (PDT) and photothermal therapy (PTT) have attracted considerable interest as a noninvasive treatment method. Photodynamic antibacterial therapy is regarded as an innovative and promising antibacterial approach due to its minor side effects and lack of drug resistance. We recently introduced a supramolecular self-assembly, NanoPcN, which realizes the combination of type I photodynamic activity and photothermal effects by modifying zinc (II) phthalocyanine with a 3-(dimethylamino) phenoxy group. Antibacterial experiments demonstrate that this “one-for-two” property endows NanoPcN with excellent antimicrobial efficacy.On the other and, photoswitchable materials have attracted considerable attention in various fields. Developing excellent solid-state dual-mode photoswitches is an important but challenging task. Herein, we propose a new strategy to construct an excited-state intramolecular proton transfer (ESIPT)-inspired photoswitches (DiAH-pht) that possesses aggregation-induced emission (AIE) feature and displays fast molecular isomerization process characterized by dual-mode behavior in the solid state.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS3-4**
[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry
Room 208+209+210 WED 14:30
Chair: Songyi Lee (Pukyung National University)

Harnessing Self-organization in Confined Soft Materials for Micro/Nanofabrication

Ashutosh Sharma

Department of Chemical Engineering, Indian Institute of Technology at Kanpur, India

Micro/nano fabrication across a variety of materials and length scales is a challenge that impacts important advances in functional interfaces, energy, electronics, health and environment. This talk will summarize some of the novel strategies pursued in our work on control of self-organization, structure formation and instabilities in highly confined soft materials such as thin films and nanofibers. The micro/nano structures created by self-organization are then applied as cell-scaffolds, biosensors, actives delivery, energy storage, nanolens and nanowire arrays to a reusable pressure sensitive adhesive.
An example of self-organized microstructures I will present is directed dewetting of thin (< 100nm).

Symposium : **KCS3-5**

[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry

Room 208+209+210 WED 15:25

Chair: Min Hee Lee (Sookmyung Women's University)

Chemical Strategies to Study Multiple Facets in Alzheimer's Disease

Mi Hee Lim

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

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid-β (Aβ) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the Aβ plaque and likely contribute to Aβ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of Aβ plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.[1-3] To find a cure for AD, we require a better understanding of the relationship between various causative factors of this devastating disease. Towards this goal, we have been developing suitable chemical tools capable of targeting and regulating multiple underlying factors or identifying the pathogenic networks composed of their direct interactions and reactivities.[4-11]References(1) *Chem. Soc. Rev.* 2012, *41*, 608.(2)*Acc. Chem. Res.* 2014, *47*, 2475; *Acc. Chem. Res.* 2021, *54*, 3930.(3)*Chem. Rev.* 2019, *119*, 1221.(4) *Proc. Natl. Acad. Sci. USA* 2010, *107*, 21990.(5) *Chem. Sci.* 2015, *6*, 1879.(6) *J. Am. Chem. Soc.* 2014, *136*, 299.(7) *J. Am. Chem. Soc.* 2015, *137*, 14785.(8) *Nat. Commun.* 2016, *7*, 13115.(9)*Proc. Natl. Acad. Sci. USA* 2020, *117*, 5160.(10) *J. Am. Chem. Soc.* 2020, *142*, 8183.(11) *Nat. Chem.* 2022, *14*, 1021-1030.

Symposium : **KCS3-6**
[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry
Room 208+209+210 WED 15:50
Chair: Min Hee Lee (Sookmyung Women's University)

Unlocking the Potential of Calcium Nanoparticles: From Bone Repair to Beyond

Elisabeth Engel*, Celia Ximenez, Joan Martí, Oscar Castaño, Soledad Pérez

IMEM-BRT- Innovation in Materials and Molecular Engineering - Biomaterials for Regenerative Therapies, Dept. Materials Science and Engineering, Technical University of Catalonia, Institute for Bioengineering of Catalonia, Barcelona, Spain

Utilization of bioactive glasses (e.g., silicates, phosphates, borates) has emerged as a potent therapeutic avenue for effecting the mending of bone fractures, fostering wound healing, and facilitating vascularization. These versatile materials exhibit a propensity for controlled dissolution within the adjacent tissue, evoking favorable bioactive responses sans the need for exogenous growth factors or cell-based interventions. This not only curtails financial burdens and averts side effects but also streamlines their translation into clinical practice.

However, the application of bioactive glasses often necessitates the inclusion of stabilizing agents (e.g., SiO44−, Ti4+, Co2+, etc.) that are not inherently abundant within the physiological milieu, and their intricate metabolic fate remains a nebulous realm. In this investigation, our focus was directed towards the synthesis of pristine calcium phosphate glasses devoid of such stabilizers. By amalgamating ethylphosphate and calcium 2-methoxyethoxide, we engendered a repertoire of nanoparticles, each characterized by distinct compositions and degradability profiles.

The production of this type of glass allows us to play with the addition of other ions to enhance nanoparticles bioactivity to tackle different tissues beyond bone.

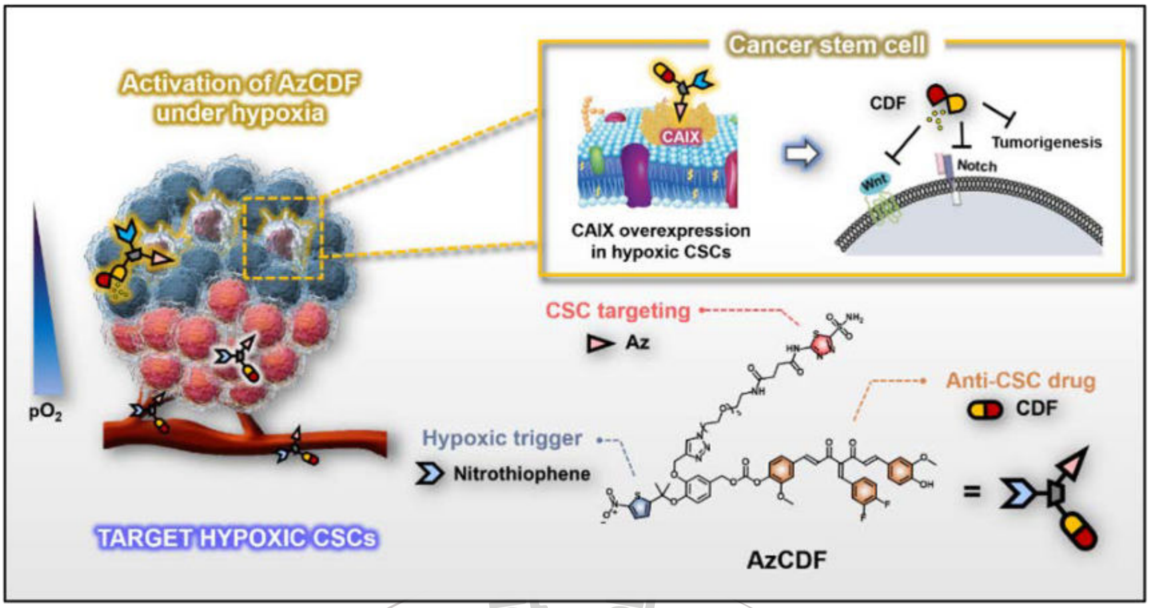
Symposium : **KCS3-7**
[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry
Room 208+209+210 WED 16:15
Chair: Min Hee Lee (Sookmyung Women's University)

Small molecule-based drug delivery system and its bioimaging

Jong Seung Kim

Department of Chemistry, Korea University, Korea

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


Activation of AzCDF under hypoxia
pO$_2$
TARGET HYPOXIC CSCs
Cancer stem cell
CAIX
CAIX overexpression in hypoxic CSCs
CDF
Tumorigenesis
Notch
Wnt
CSC targeting
Az
Anti-CSC drug
CDF
Hypoxic trigger
Nitrothiophene
AzCDF
=

Symposium : **KCS3-8**

[KCS-ACS Applied Bio Materials Research Publications Summit] Research Trends and Challenges in Nano-bio Chemistry

Room 208+209+210 WED 16:40

Chair: Min Hee Lee (Sookmyung Women's University)

Resources at ACS for Career Advancement of South Korean STEM Professionals

Deeksha Gupta

American Chemical Society, United States

This session will highlight the array of resources available with the American Chemical Society (ACS) aimed at fostering the career growth of South Korean STEM professionals at every career stage. These resources encompass various avenues such as the Global Virtual Symposia that enable researchers to present their work on a global stage. Additionally, the Faculty Leadership Summit provides a platform for early career faculty to enhance both their academic and leadership proficiencies. Further offerings include the ACS Author Lab, designed to refine manuscript writing skills among the newly admitted PhD students, and Virtual Internship Capsule modules geared towards upskilling of the undergraduate and masters' students to enhance their industry readiness. Collectively, these resources and several more contribute to a comprehensive framework for advancing the careers of South Korean STEM professionals, allowing them to build networks to facilitate collaboration and innovation, and showcase the very best of Korean Chemical sciences research with the world.

Symposium : **KCS4-1**
[IBS Symposium] Carbon and Related Materials
Room 211+212+213 WED 13:00
Chair: Rodney S. Ruoff (IBS / UNIST)

How’s your interface?

Rodney S. Ruoff

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS; located at the UNIST Campus)/, Department of Chemistry and Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST), Korea

The type of interface(s) formed between adjacent materials A and B can vary depending on A and B and parameters such as temperature and pressure—among other parameters. Qualitative terms such as “chemisorption” (covalent bonding) and “physisorption” (van der Waals bonding and perhaps including H-bonding in the minds of some and not others) are used to convey the type of bonding present at the interface. I will discuss several interfaces that interest me and my team—and how I think about these interfaces as opening new opportunities for the growth of certain types of materials.

We appreciate support from the Institute for Basic Science (IBS-R019-D1).

Symposium : **KCS4-2**
[IBS Symposium] Carbon and Related Materials
Room 211+212+213 WED 13:40
Chair: Rodney S. Ruoff (IBS / UNIST)

MINE-based (Molecular Integration NanoscopE-based) Closer Look into Materials and Beyond.

Yung Doug Suh

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

Just like the Nuclear Magnetic Resonance (NMR) has won two individual Nobel Prizes in Chemistry, and then eventually went to real world application of Medical MRI, while Femtosecond Spectroscopy, Biopolymer Mass Spectrometry, Super-Resolution Nanoscopy, as well as Cryo TEM have won the Nobel Prize in Chemistry, these kind of "New Chemical Measurement Methods" have been playing a central role in the "discovery and application of entirely new materials" that I call here as "Mining". Starting from the original Raman-MINE (Molecular Integration NanoscopE) in 2005, we have "mined" the gold silver nano dumbbell (GSND) nanoparticles (2010 Nature Materials: >1,200 citations), the Gold Nano Droplet (GND) nanoparticles (2011 Nature Nanotechnology: >1,000 citations), we have reached up to the new class of materials names as Photon Avalanche Nano Particles (Photon ANP) (Jan 14th , 2021 Nature Cover Article) based on an appropriate type of MINEs for each different cases. "MINE-based Mining" with single molecule/single particle detectionsensitivity, can be customized in various forms according to the characteristics of the new materials to be "mined": different materials can be "mined" using appropriate selection & combination of incident light & detection light pathways and imaging modes. In this presentation, I will talk about how to apply this MINE to the carbon materials and beyond.

Symposium : **KCS4-3**

[IBS Symposium] Carbon and Related Materials

Room 211+212+213 WED 14:30

Chair: Rodney S. Ruoff (IBS / UNIST)

Hexagonal and amorphous boron nitride thin films

Hyeon Suk Shin

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

Hexagonal boron nitride (hBN) is a promising two-dimensional (2D) material owing to its unique optical properties in the deep-UV region, mechanical robustness, thermal stability, and chemical inertness. hBN thin films have gained significant attention for various applications, including nanoelectronics, photonics, single photon emission, anti-corrosion, and membranes. Thus, wafer-scale growth of hBN films is crucial to enable their industrial-scale applications. In this regard, chemical vapor deposition (CVD) is a promising method for scalable high-quality films. To date, considerable efforts have been made to develop continuous hBN thin films with high crystallinity, from those with large grains to single-crystal ones, and to realize thickness control of hBN films by CVD. However, the growth of wafer-scale high crystalline hBN films with precise thickness control has not been reported yet. The hBN growth is significantly affected by substrate, in particular the type of metals, because the intrinsic solubilities of boron and nitrogen depend on the type of metal. In this talk, state-of-the-art strategies adopted for growing wafer-scale, highly crystalline hBN are summarized, followed by the proposed mechanisms of hBN growth on catalytic substrates [1]. Furthermore, various applications of the hBN thin films are demonstrated, including a dielectric layer, an encapsulation layer, a wrapping layer of gold nanoparticles for surface enhanced Raman scattering, a proton-exchange membrane, a template for growth of other 2D materials or nanomaterials, and a platform of fabricating in-plane heterostructures. In addition, amorphous BN (aBN) as a counterpart of crystalline hBN is introduced [2]. Detailed structural characterisation indicates that a-BN is sp2-hybridised, with no measurable crystallinity, and mechanically robust, with excellent diffusion-barrier characteristics. The aBN thin film shows ultra-low dielectric constant (< 2.5), indicating great potential for its applications in Cu interconnects of integrated circuits. [1] K. Y. Ma et al., Nature 606, 88 (2022).[2] S. Hong et al., Nature 582, 511 (2020).

Symposium : **KCS4-4**
[IBS Symposium] Carbon and Related Materials
Room 211+212+213 WED 15:10
Chair: Rodney S. Ruoff (IBS / UNIST)

Computational/theoretical analysis of various carbon-related materials

Seung Kyu Min

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

In this presentation, I will provide several computational research works focused on carbon-related materials, conducted in conjunction with experimental efforts. Initially, I will outline the investigation into proton affinity (PA) and gas phase basicity (GPB) of a selection of diamondoid molecules. This exploration is driven by the goal of ascertaining the feasibility of incorporating an additional hydrogen atom or proton within a molecule. Given the spatial limitations of the interstitial site within cubic diamondoids, only a proton holds potential for accommodation in such confined spaces. The presentation will include depictions of molecular structures, along with PA and GPB values, derived from density functional theory (DFT) calculations. Notably, specific diamondoids exhibit behavior akin to a "superbase." The subsequent part of the presentation will delve into a collaborative effort of computational and experimental approaches, aiming to comprehend the mechanisms of the formation of graphite intercalation compounds (GICs). Experimental endeavors have yielded a pristine stage-1 GIC intercalated with trifluoroacetic acid (CF_3COOH), designated as CF_3COOH-GIC, synthesized via electrochemical oxidation. Employing a DFT analysis encompassing diverse atomic configurations of materials, the intercalation processes will be elucidated. Furthermore, the presentation will highlight theoretical and computational methodologies employed to elucidate coupled electron-nuclear dynamics within materials. These approaches enable real-time simulations to unravel the propagation of electrons or holes within materials.[1] Camacho-Mojica, D. et. al., Phys. Chem. Chem. Phys., 24, 3470-3477, 2022[2] Gurzęda, B. et. al., Chem. Mater., 23, 217-231, 2021

Symposium : **KCS4-5**

[IBS Symposium] Carbon and Related Materials

Room 211+212+213 WED 15:40

Chair: Rodney S. Ruoff (IBS / UNIST)

DFT modeling of carbon transformation through dissolution in metal

Geunsik Lee

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

Carbon is commonly dissolved in late transition metal solids by occupying the interstitial sites. This provides a way to find a reaction pathway from one carbon reactant to another carbon containing products. Here, we present a previous work of finding reaction mechanims by DFT modeling and calculations, associated with the key rate limiting steps, explaining the experimentally measured reaction rates through dissolution of diamond into Ni or Co. Further, recent extension of the previous modeling to different types of metal will be presented, thus providing key insight to design a metal to grow a desired form of carbon. We appreciate support from the Institute for Basic Science (IBS-R019-D1).

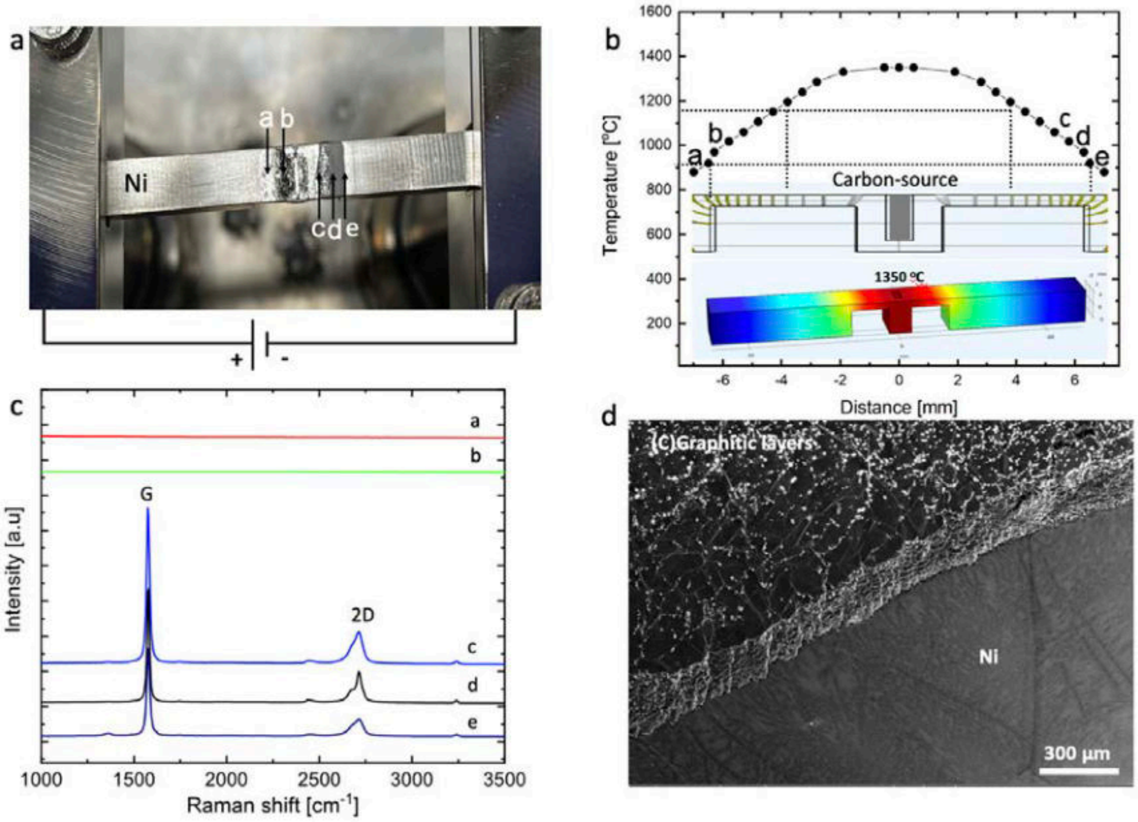
Symposium : **KCS4-6**
[IBS Symposium] Carbon and Related Materials
Room 211+212+213 WED 16:30
Chair: Rodney S. Ruoff (IBS / UNIST)

Fractionation of carbon isotopes using electromigration in high carbon solubility metals

Alisher Sultangaziyev, Sun Hwa Lee[1], Dongho Jeon[1], Da Luo[2], Won Kyung Seong[1,*], Rodney Ruoff[3,*]

Chemistry, Institute for Basic Science (IBS), Center for Multidimensional Carbon Materials (CMCM), Korea
[1] *Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*
[2] *Institute for Basic Science, Korea*
[3] *Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

We have studied the isotope fractionation of carbon (C) atoms using electromigration and a controlled temperature gradient near the eutectic temperature of cobalt (Co) and nickel (Ni) at 1300 °C and gradient in the nearby region to 800 °C. Electromigration involves the movement of (in this case carbon) atoms within metals as energy is transferred to the carbon atoms, inducing their migration (in our case here) toward the negative electrode. A carbon source was placed within cobalt and nickel bars at the center of machined pockets. The temperature gradient of the Co and Ni bars was measured using a pyrometer and simulated through Comsol. We generated an electromigration and temperature gradient within the Co and Ni bars by employing a Joule heating method with either DC or AC. The carbon source dissolved entirely within 30 hours. Raman spectroscopy revealed carbon precipitation concentrated near the 900 °C region of the negative electrode for both the Co and Ni bars, a phenomenon attributed to electromigration effects; no carbon precipitated anywhere from the centerline towards the positive electrode with DC. For AC, a symmetric distribution of precipitated carbon was observed. For the various isotope ratios of 12C/13C of the carbon source, we observed a higher occurrence of 12C-rich graphite precipitated on the Ni bar than on the Co bar. We appreciate support from the Institute for Basic Science (IBS-R019-D1).


a
Ni
a b
c d e
+
-
b
Temperature [ºC]
1600
1400
1200
1000
800
600
400
200
Carbon-source
1350 ºC
a
b
c
d
e
-6
-4
-2
0
2
4
6
Distance [mm]
c
Intensity [a.u]
a
b
G
2D
c
d
e
1000
1500
2000
2500
3000
3500
Raman shift [cm-1]
d
(C)Graphitic layers
Ni
300 μm

Symposium : **KCS4-7**

[IBS Symposium] Carbon and Related Materials

Room 211+212+213 WED 16:50

Chair: Rodney S. Ruoff (IBS / UNIST)

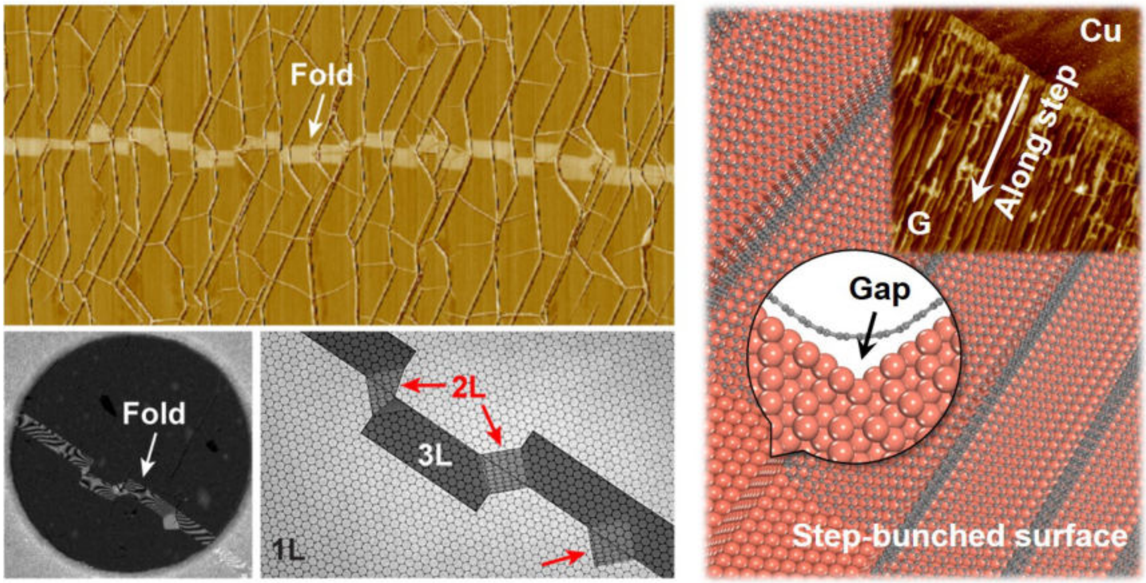
Interfacial properties about single crystal graphene grown on Cu(111) surfaces

Da Luo[*], Meihui Wang, Rodney Ruoff[1,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials, IBS CMCM / UNIST, Korea*

Epitaxial growth by chemical vapor deposition (CVD) on single crystal Cu(111) surfaces is effective to make single crystal graphene films over large areas. We grew high-quality single crystal graphene on “home-made” Cu(111) foil surfaces and studied the interfacial properties including self-folding of graphene and the diffusion of water molecules at the graphene-Cu interface. We found long and parallel graphene folds (with a thickness of 3 graphene layers) spontaneously formed in CVD-grown single-crystal graphene film; their formation is triggered by the anisotropic relaxation of interfacial stress due to the formation of highly ordered bunched Cu steps under the graphene. Such folds are fractured into “back-and-forth” patterns at bunched Cu step edge regions because compressive stress (as we learned) is concentrated at such regions, with cracks propagating along only zigzag and/or armchair directions. We found that even as-grown epitaxial single crystal graphene cannot protect the underlying Cu(111) surface from wet-oxidation because there always exists a diffusion pathway for water to laterally diffuse under the graphene from edges: a “physical gap” exists between the monolayer graphene and the bunched Cu step ‘corners’ at such edges. This interfacial diffusion of water is completely eliminated if ultra-flat graphene is coating an ultrasmooth Cu(111) surface. We thus discovered/showed how to precisely control both the structures and properties of graphene by controlling the interface structures. Our studies may shed light on the controllable synthesis and property modulation of other two-dimensional materials. We appreciate support from the Institute for Basic Science (IBS-R019-D1).


Fold
Fold
2L
3L
1L
Cu
Along step
G
Gap
Step-bunched surface

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **KCS4-8**

[IBS Symposium] Carbon and Related Materials

Room 211+212+213 WED 17:10

Chair: Rodney S. Ruoff (IBS / UNIST)

Putty-like gallium: A simple approach to forming gallium composites

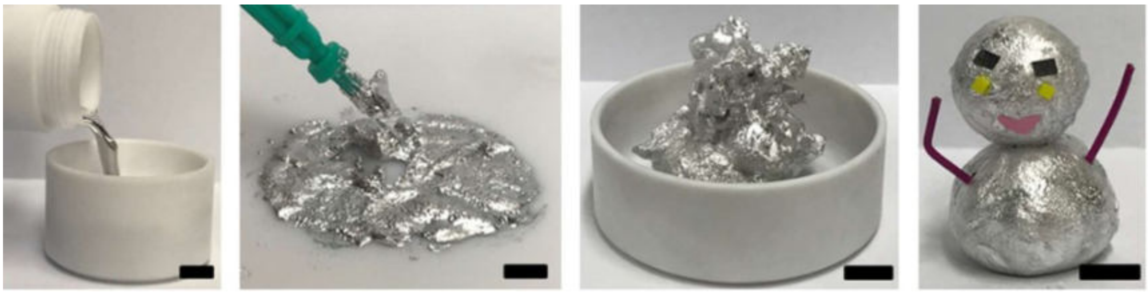
Benjamin Cunning[*], **Yan Gong, Rodney Ruoff**[1,*]

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS; located at the UNIST campus), Korea

[1]*Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS; located at the UNIST campus)/, Department of Chemistry, UNIST / Department of Materials Science and Engineering, UNIST, Korea*

We report [1] a versatile method to make liquid metal putty-like composites by vigorously mixing gallium (Ga) with non-metallic particles of graphene oxide (G-O), graphite, diamond, and silicon carbide that display either paste or putty-like behavior depending on the volume fraction. Unlike Ga, the putty-like mixtures can be kneaded and rolled on any surface without leaving residue. By changing temperature, these materials can be stiffened, softened, and, for the G-O–containing composite, even made porous. The gallium putty (GalP) containing reduced G-O (rG-O) has excellent electromagnetic interference shielding effectiveness. GalP with diamond filler has excellent thermal conductivity and heat transfer superior to a commercial liquid metal–based thermal paste. Composites can also be formed from eutectic alloys of Ga including Ga-In (EGaIn), Ga-Sn (EGaSn), and Ga-In-Sn (EGaInSn or Galinstan). We also report an extension of this work in which putty-like gallium can be prepared with vigorous mixing in air that allows incorporation of any filler. In this form the gallium can be used to conveniently prepare alloy melts, and solid porous alloys of gallium; We appreciate support from the Institute for Basic Science (IBS-R019-D1). [1] Chunhui Wang, Yan Gong, Benjamin V. Cunning*, Seunghwan Lee, Quan Le, Shalik R. Josh, OnurBuyukcakir, Hanyang Zhang, Won Kyung Seong, Ming Huang, Meihui Wang, Jaeseon Lee, Gun-Ho Kim, Rodney S. Ruoff. Science Advances, 7, eabe3767, 2021.

Figure 1. Photos showing liquid gallium transitioning from a liquid to a thick slurry, and to a malleable putty. The metallic putty is highly processable and versatile, it can be molded into a variety of shapes.



Symposium : **KCS4-9**

[IBS Symposium] Carbon and Related Materials

Room 211+212+213 WED 17:30

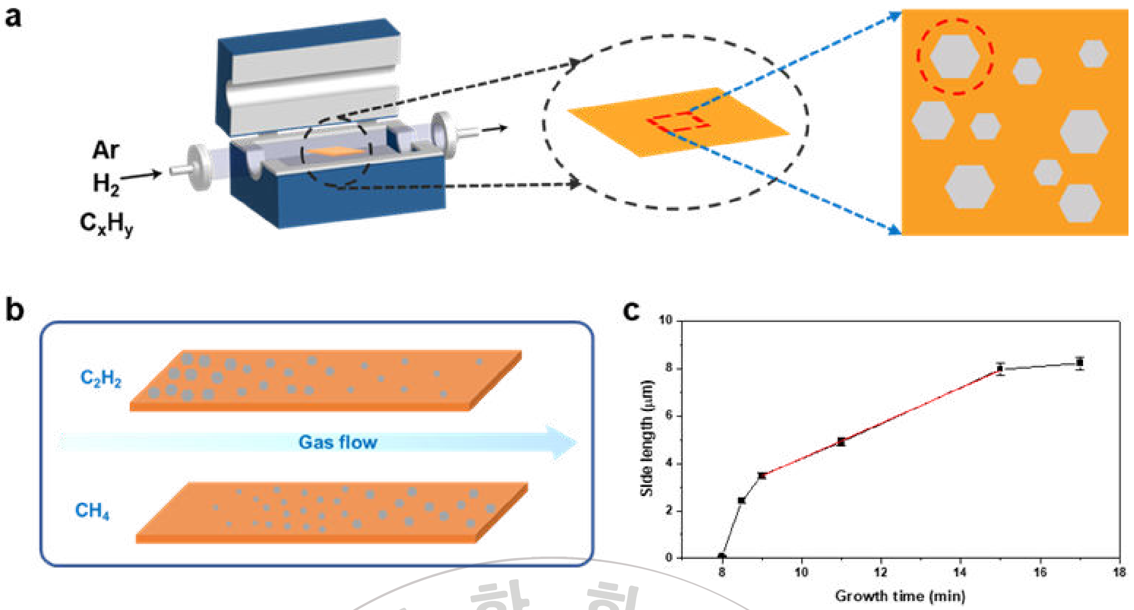
Chair: Rodney S. Ruoff (IBS / UNIST)

The growth kinetics of graphene islands on Cu(111) foils using C_2H_2, C_2H_4, C_2H_6, and CH_4 as reagents

Meihui Wang, Da Luo, Geunsik Lee[1], Rodney Ruoff[2,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*
[2]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

Chemical vapor deposition of CH_4 on Cu-based substrates at above 1270 K is currently a typical route for the scalable synthesis of large-area high-quality single-layer graphene (SLG) films. However, the controllable preparation of high-quality single-crystal SLG films at lower temperatures is challenging, due to the low activities of CH_4 and Cu. We have described our use of C_2H_4 and Cu-Ni(111) foils as the carbon precursor and the substrate, respectively, and achieving large area fold-free single-crystal SLG films at 1000-1030 K. This method suppresses the formation of graphene folds (one kind of graphene wrinkle) and yields graphene films with uniform electronic properties.[1] Here, we study the growth kinetics of graphene islands on Cu(111) foils by using CH_4, C_2H_6, C_2H_4 and C_2H_2, respectively. We find that CH_4 shows a different growth behavior than C_2H_6, C_2H_4 and C_2H_2 (which show similar growth behavior). We will describe a reliable method to measure the 'apparent activation enthalpy' (Eapp) of the graphene growth process and find that C_2H_2 shows the lowest Eapp value. By using C_2H_2 as the carbon precursor, we achieve high-quality single-crystal adlayer-free SLG films on Cu(111) foils at 1170 K. We appreciate support from the Institute for Basic Science (IBS-R019-D1).[1] Wang, M.; Huang, M.; Luo, D.; Li, Y.; Choe, M.; Seong, W. K.; Kim, M.; Jin, S.; Wang, M.; Chatterjee, S.; Kwon, Y.; Lee, Z.; Ruoff, R. S. Nature 2021, 596 (7873), 519-524.


a
Ar
H_2
C_xH_y
b
C_2H_2
Gas flow
CH_4
c
Side length (μm)
0
2
4
6
8
10
Growth time (min)
8
10
12
14
16
18

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **KCS5-1**
[Chemistry Symposium for Future Innovation] The Role of Chemistry in Materials Innovation for Sub-nm Semiconductors
Room 214 WED 13:00
Chair: Hyun-Dam Jeong (Chonnam National University)

Advancements and State-of-the-Art Trends in Semiconductor Photoresist Materials

Sang Jun Choi

Chempole Co., Ltd, Korea

The semiconductor industry has continually evolved, driven in part by advancements in lithography technology. The advent of the AI era has further underscored the importance of this technology. Concurrently, the significance of photoresist materials in semiconductor lithography has grown, acting as a key determinant in the industry's technological roadmap. With the recent adoption of Extreme Ultraviolet (EUV) technology, the focus on photoresist materials has intensified, and research in this area is notably active. In this presentation, I will explore the evolving nature of these resist materials, discuss the characteristics of various photoresist types, and highlight the emerging importance of EUV photoresist material. Continued research and investment in these crucial photoresist materials will play a pivotal role in propelling the semiconductor industry, and by extension, the AI era, forward.

Symposium : **KCS5-2**

[Chemistry Symposium for Future Innovation] The Role of Chemistry in Materials Innovation for Sub-nm Semiconductors

Room 214 WED 13:30

Chair: Hyun-Dam Jeong (Chonnam National University)

Development of selective dissociating PECVD process for ultra low-k film

Jung Hyung Kim

Advanced Instrumentation Institute, Korea Research Institute of Standards and Science, Korea

In this study, we have developed a process that reduces the dielectric constant of thin films by introducing the concept of selective bond breaking, wherein only desired bonds of the precursor are broken to form the film. To achieve selective dissociation of the precursor, we controlled the plasma electron temperature and density. We investigated the impact of electron density and electron temperature on the reduction of the dielectric constant in SiCOH thin films, utilizing dimethyldimethoxysilane (DMDMS) as a precursor, at various pressures. The measured electron density and electron temperature decreased with increasing pressure, with the decrease in electron density attributed to local electron kinetics. Additionally, the reduced electron temperature was a result of increased inelastic collisions between electrons and neutral species in the chamber. Quadrupole mass spectroscopy revealed that CH3 radicals experience less dissociation from DMDMS molecules at higher pressures. Fourier transform infrared spectroscopy confirmed an increase in Si-CH3 bonds in SiCOH thin films at higher pressures. As a result, the dielectric constant and refractive index of the SiCOH films were reduced at low electron density and electron temperature.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS5-3**
[Chemistry Symposium for Future Innovation] The Role of Chemistry in Materials Innovation for Sub-nm Semiconductors
Room 214 WED 14:00
Chair: Hyun-Dam Jeong (Chonnam National University)

Molecules for Electronics Applications

Hyo Jae Yoon

Department of Chemistry, Korea University, Korea

Molecular chemistry plays a crucial role in modern electronics applications, as electronic devices continue to be miniaturized into the molecular scale. Additionally, the semiconductor industry now deals with objects smaller than 10 nm. This presentation aims to highlight the significant contributions of molecular chemistry to electronics applications and the semiconductor industry. The first part of the presentation focuses on the exploitation of N-heterocyclic chemistry. It demonstrates how the N-heterocyclic chemistry can be utilized to design molecular diodes and enhance our understanding of charge tunneling via molecular orbitals. Moving on to the second part, the presentation showcases the contributions of organometallic and supramolecular chemistries to the development of extreme ultraviolet (EUV) photoresists used in the photolithography process of the modern semiconductor industry. In conclusion, this presentation underscores that, by leveraging well-established synthetic chemistry, one can gain the ability to tailor atomic structures of individual molecules in designing efficient active materials for electronics applications.

Symposium : **KCS5-4**
[Chemistry Symposium for Future Innovation] The Role of Chemistry in Materials Innovation for Sub-nm Semiconductors
Room 214 WED 14:40
Chair: Hyo Jae Yoon (Korea University)

Optical properties of materials and components used in EUVL Materials

Chan-Cuk Hwang

Pohang Accelerator Laboratory, Korea

EUV lithography is a key technology in semiconductor device fabrication. The super expensive EUV scanner can only be manufactured by ASML in the Netherlands. Materials and components, such as EUV photoresist, EUV source, mirror, filter, mask, pellicle, and metrology are rapidly under development in the world. I would like to talk about key technologies needed to build a EUV industrial ecosystem in south korea and what I have been doing until now.

Symposium : **KCS5-5**
[Chemistry Symposium for Future Innovation] The Role of Chemistry in Materials Innovation for Sub-nm Semiconductors
Room 214 WED 15:10
Chair: Hyo Jae Yoon (Korea University)

Development of materials based on electron-driven chemistry for sub-nm node semiconductors

Hyun-Dam Jeong

Department of Chemistry, Chonnam National University, Korea

In-depth research in the field of chemistry is imperative for the innovation of materials used in sub-nm node semiconductors and AI semiconductors. An integration of quantum chemistry, materials chemistry, synthetic chemistry, and photoelectron spectroscopy is essential. Comprehensive research on fundamental scientific issues related to the elucidation of the correlation between the molecular structure of materials and their properties/functions is necessary. Our material design for semiconductor materials is currently constrained due to an incomplete understanding of the electron-molecule collision mechanism. Extreme Ultraviolet Lithography (EUVL) has risen as a pivotal technology for fabricating advanced semiconductor devices that prioritize both resolution and performance. In comparison to conventional organic resists, inorganic resists demonstrate superior etch resistance. This study introduces the design and progression of inorganic resists for EUVL, anchored in electron-driven chemistry. By employing ab initio calculations to analyze bond dissociation within the molecules of a tin compound resist, we could anticipate the products formed during the collision of the resist molecule with secondary electrons generated by EUV irradiation. Additionally, we could predict the condensation reactions of Sn-OH groups. For 0.7 nm node logic semiconductors anticipated in 2023, a low-k material with a dielectric constant of 2.2 is essential. In the PECVD process to form a low-k film, the potential for controlling dielectric constants and mechanical properties through the selective bond dissociation of precursors is being highlighted. For a clear understanding of this, the amalgamation of electron-driven and quantum chemistry is indispensable.

Symposium : **KCS6-1**

[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach

Room 301 WED 14:00

Chair: Doo-Hyun Ko (Sungkyunkwan University)

Segmental dynamics of a component polymer in multicomponent polymer mixtures

Keewook Paeng

Department of Chemistry, Sungkyunkwan University, Korea

Due to their ease of production and ability to modify properties through mixing different components, polymer-containing mixtures, such as small molecules dispersed in a polymer matrix and polymer blends, are used in a variety of applications, including photoresists and solid polymer electrolytes. In understanding these multicomponent mixtures, which are mostly amorphous materials, the dynamics leading to the glass transition are crucial since the glass transition determines the integrity of the materials, and unlike thermodynamic transitions, a kinetic process. Understanding the dynamics of a component in a mixture is even more pivotal because many applications use mixtures rather than single-component systems, and the performance of these systems depends on the mobility of each component. Here, the reorientation of a polymer-tethered fluorescent probe was utilized to examine the segmental dynamics of a near-infinitely diluted component polymer in polymer blends near the glass transition. Unexpectedly, it is found that the dynamics of a dilute component follow that of the other component's temperature dependence with a temperature shift that may result from a local composition of a 10% dilute component. On the other hand, the local dynamic environment of the dilute component can become either as heterogeneous as a component that is more inherently heterogeneous or more heterogeneous than both regardless of which polymer is diluted.

Symposium : **KCS6-2**
[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach
Room 301 WED 14:30
Chair: Doo-Hyun Ko (Sungkyunkwan University)

Understanding Chemical Reactions of Cellulose at High Temperatures and Employing Pretreatments for Carbon Fiber Production

Sung-Soo Kim

Carbon Composite Materials Research Center, Korea Institute of Science and Technology, Korea

Polyacylonitrile (PAN)-based fibers have been widely used as a precursor for the fabrication of high-performance carbon fibers (CFs), which can be applied in aerospace, sporting goods, and automobile industries due to their superior specific strength. However, one of the most prominent issues related to PAN-based CFs is their high fabrication cost. As more than half of the total cost of manufacturing PAN-based CF is represented by the PAN precursor, other polymeric materials have been investigated and utilized as an alternative precursor to fabricate cost-effective CFs.Cellulose, which consists of linear chains of β-1,4-linked d-glucose units, has been considered as biorenewable and low-cost precursors for the production of CFs. Various natural cellulose fibers have been extensively utilized as a source of textile fibers throughout human history. However, one major issue associated with the cellulose pyrolysis arises from side reactions that release volatile substances, leading to a low char yield after carbonization and poor mechanical properties of the resulting CFs.In this work, we demonstrate that both pretreatments with sulfuric acid and electron beam irradiation can significantly increase the char yield for the fabrication of cellulose-derived CFs. Our experimental results and previous studies on the mechanism of cellulose pyrolysis mutually indicate that sulfuric acid and electron beam effectively induced the fragmentation of cellulose chains, which plays a significant role in augmenting the char yield after subsequent carbonization as well as reducing the time for thermostabilization by a factor of 10. The resulting CFs exhibited measurable mechanical properties, in stark contrast to the inherently brittle CFs generated without these pretreatments.

Symposium : **KCS6-3**
[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach
Room 301 WED 15:00
Chair: Doo-Hyun Ko (Sungkyunkwan University)

Simulation Studies on Mechanical Properties of Elastomers for Various Applications

Bong June Sung

Department of Chemistry, Sogang University, Korea

Entropy determines not only the direction of a particular spontaneous process but also the various physical properties of materials systems. For example, the configurational entropy determines either the pressure of a gaseous system or the miscibility of liquid mixtures (including complex polymeric liquid mixtures). Similarly, the conformational entropy of a polymer chain determines the shear modulus of polymer networks (or elastomers) such that the shear modulus of the elastomers should be inversely proportional to the degree of polymerization of the polymer chains. Therefore, when designing and developing new elastomers for various applications (such as thermoplastic elastomers and stretchable polymer semiconductors), it is of crucial importance to understand that the entropy should play a critical role in regulating the mechanical properties. In this talk, I will present recent molecular simulation studies in my research group to understand the mechanical properties of polymer mixtures and block copolymers, and will also discuss how the entropy will contribute to those mechanical properties.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS6-4**
[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach
Room 301 WED 15:30
Chair: Doo-Hyun Ko (Sungkyunkwan University)

Entropy Engineering for Polymers

Youngjong Kang

Department of Chemistry, Hanyang University, Korea

Over the past century, significant progress has been made in understanding the physical properties of polymers, leading to a certain level of maturity in the field. This progress has been driven by innovative synthetic techniques, precise experimentation, and profound physical insights. However, despite the widespread use of enthalpy-based approaches, such as controlling chemical structures, bonding, and molecular interactions, there has been little active effort to exploit polymer properties by manipulating entropy.In this presentation, I will delve into the role and importance of entropy control in various studies of polymer properties, such as crystallization, blending, and phase transition. Especially a novel concept named “entropy diluent”, which can substantially decrease the conformational entropy of polymer chains, will be extensively discussed.

Symposium : **KCS6-5**

[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach

Room 301 WED 16:20

Chair: Bong June Sung (Sogang University)

Entropy-driven strategy to suppress organic phase separation

Doo-Hyun Ko

Department of Chemistry, Sungkyunkwan University, Korea

Organic photovoltaics (OPVs) possess unique properties that hold significant promise for emerging applications, such as those in the Internet of Things (IoT). The long-term stability of OPVs stands as a critical factor determining their practicality in commercial fields. In addition to their ability to harness solar light, OPVs should be designed to operate under various irradiation conditions to ensure continuous power generation for 24 hours. In this study, we present multi-component OPVs that simultaneously enhance efficiency and prolong their operational lifetimes. These multi-component blends exhibit an extended spectral response range and an improved charge transport process, effectively suppressing recombination. This results in high output power, suitable for powering low-power electronic devices. Furthermore, the multi-component blend notably reduces the aggregation of meta-stable molecules. The combination of heightened efficiency, extended device lifetimes, and the utilization of multi-component blends holds promise for commercially viable OPVs across diverse applications.

Symposium : **KCS6-6**
[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach
Room 301 WED 16:50
Chair: Bong June Sung (Sogang University)

Apex-dependent supramolecular assemblies from 2G dendron mesocrystals

Du Yeol Ryu*, Woo-Dong Jang[1], Byeongdu Lee[2]

Chemical and Biomolecular Engineering, Yonsei University, Korea
[1]*Department of Chemistry, Yonsei University, Korea*
[2]*Advanced Photon Source, Argonne National Laboratory, United States*

The observation of unique arrays and alignments assembled by new ordered structures facilitates the study of structure-property relationships and the development of functional materials. In the past two decades, the fascinating sphere-packing Frank-Kasper (FK) phases have come to us as an intriguing molecular assembly. Well-studied soft-matter systems for self-assembly include small-molecular components of dendrons, surfactants, liquid crystals, and block copolymers. Among those candidates, the dendrons show the modular structures that can pack into ordered structures with complex 2D and 3D geometries, enabling potential applications in the fields of molecular electronics, catalysts, porous materials, drug delivery, and bio-mimetic systems. In this study, we design and present a strategy to create the FK phases from simple second-generation (G2) dendrons possessing different apex functionalities (Xs) that modulate core interactions among the apex groups. The dendrons of G2-X were synthesized by a convergent method and post-functionalized at terminal X to have CONH2, CH2OH, and CH2NH2 which are in decreasing order of core interactions (or H-bonding). With a versatile modular platform of G2-X, we seek to answer a question about how enthalpic and entropic contributions affect dendron assemblies.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS6-7**
[Chemistry Symposium for Future Innovation] High-performance Multicomponent Macromolecular Materials with an Entropy Approach
Room 301 WED 17:20
Chair: Bong June Sung (Sogang University)

Ion transport in advanced polymer electrolytes: role of morphology and interface

Chang yun Son

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

Electrostatic interactions plays a dominant role in charged materials systems. Understanding the complex correlation between macroscopic properties with microscopic structures is of critical importance to develop rational design strategies for advanced materials. But the complexity of this challenging task is augmented by interfaces present in the system, requiring a multi-scale approach to incorporate the spatiotemporal resolution needed for molecular descriptors and the interfacial heterogeneity.In this talk, I'll present our ongoing efforts to enable predictive molecular simulations of these highly charged systems, especially focusing on the field of developing advanced polymer electrolytes. A key advancement has been made with the development of predictive multi-scale force field for ionic liquids (ILs) and polymers based entirely on first-principle calculation. New physical insights gained from the new simulation model and simulation algorithms will be discussed, which includes simulation study of lithium ion transport under nanoscale confinement formed by microphase separation, and controlling morphology and interfaces to enhance the mechanical and dynamic properties of novel polymer-IL mixture system for energy application.

Symposium : **KCS7-1**
[KCS] Special Symposium for Young Chemists
Room 302+303 WED 13:00
Chair: Tae Kyu Kim (Yonsei University)

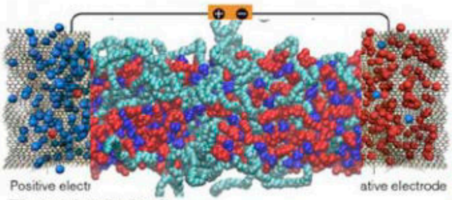
Controlling Charged Interfaces for Energy/Bio Applications: Insights from Predictive Molecular Simulations

Chang yun Son

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

Electrostatic interactions plays a dominant role in charged materials systems. Understanding the complex correlation between macroscopic properties with microscopic structures is of critical importance to develop rational design strategies for advanced materials. But the complexity of this challenging task is augmented by interfaces present in the charged materials systems, such as electrode-electrolyte interfaces or biological membranesIn this talk, I'll present our ongoing efforts to enable predictive molecular simulations of these highly charged systems. Two major advances will be highlighted – the development of predictive multi-scale force field for ionic liquids (ILs) and polymers based entirely on first-principle calculations, and the development of simulation algorithms to treat surface polarization and proper thermal equilibrium in polarizable MD simulations. New physical insights gained from the new simulation model and simulation algorithms will be discussed, which includes polarization effects on the ion adsorption at air/water and water/electrode interfaces, as well as a sophisticated design of polymer electrolytes for next generation energy storage material with tailored structural and dynamic properties.Another important study investigates the molecular transport of synthetic molecules across the lipid membrane, representing complex interfacial systems abundant in biology. Our critical analysis brings two prominent field of energy materials and biological science under common perspective, to stimulate crossover in both research field that have been largely separated.

Predictive molecular models of *charged interfaces*

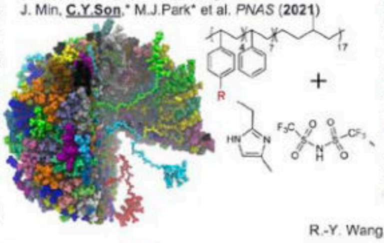


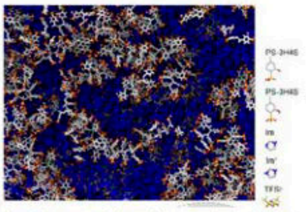
Electrochemical cell

C.Y. Son, Z.-G. Wang *PNAS* (2021), M. Salanne, *Top Curr Chem (Z)*

Soft matter self-assembly

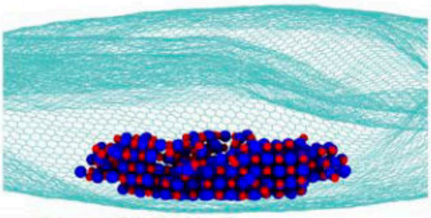
J. Min, **C.Y.Son**,* M.J.Park* et al. *PNAS* (**2021**)





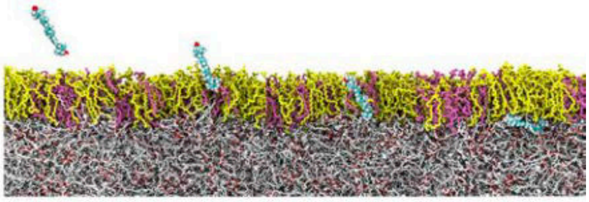
Ion trasnport in polymer electrolytes

R.-Y. Wang, **C.Y.Son**,* M.J.Park* et al. Adv. Mater. (**2022**)



Nanoparticle growth in liquid cell

J. Hong, **C.Y.Son**,*, Y.Yang*, Y.-S.Lee*, S.J.Yoo*, D.W.Chun* *et al. Nature.* (2022)



Biological membranes

S.H. Son, **C. Y.Son***, S.S. Oh*, J.Y. Lee* *et al, Nat. Commun.* (2022)

Symposium : **KCS7-2**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 13:25

Chair: Tae Kyu Kim (Yonsei University)

Manipulating Light, Matter, and Energy for Carbon Fixation

Sungju Yu

Department of Chemistry, Ajou University, Korea

Gold nanoparticles exhibit the capability to activate small molecules by efficiently absorbing light energy within the visible-frequency spectrum. These interactions, termed localized surface plasmon resonances (LSPRs), entail the coordinated oscillations of electrons within metal nanoparticles. This presentation initiates by examining the photochemical effects prompted by LSPR excitation, highlighting its role in driving the disintegration of molecular bonds and the creation of energy-dense compounds, like hydrocarbons sourced from carbon dioxide. Notably, in contrast to electrochemical pathways where hydrocarbon formation on gold surfaces is hindered, LSPR-driven processes showcase distinct attributes, promoting multi-electron reduction and directing product formation towards hydrocarbons. The rate of reaction and the branching of products depend on the light energy and flux. Through an amalgamation of theoretical models and experimental validation, we discuss the conversion of photon energy into molecular chemical bonds. Additionally, we delve into the emergence of novel intermediates, pathways, and product distributions on plasmonic nanoparticles, elucidating the intriguing phenomena underpinning these unconventional reactivity patterns.

Symposium : **KCS7-3**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 13:50

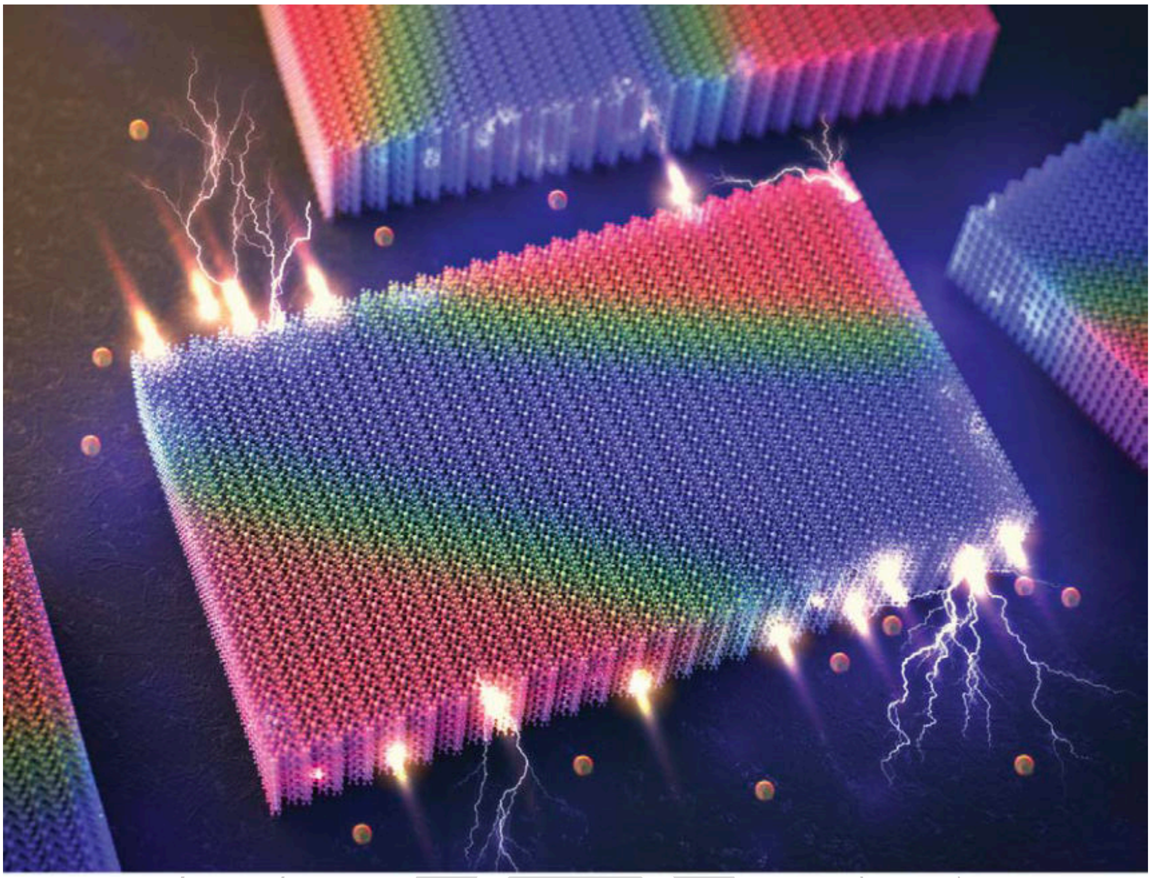
Chair: Tae Kyu Kim (Yonsei University)

How interfaces control lithium (de)insertion pathway: liquid electrolyte and solid electrolyte

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

In the realm of lithium-ion batteries, the process of lithium (de)insertion follows a two-fold pathway. This pathway encompasses (1) charge transfer occurring at the electrolyte-electrode interface, and (2) solid-state lithium diffusion within the electrode. Historically, these two transport mechanisms have been regarded as distinct and investigated separately, owing to their sequential occurrence during battery cycling. However, our recent research demonstrates that the kinetics of charge transfer can influence the spatial distribution of lithium on the surface, consequently affecting the entire lithium (de)insertion pathway. Furthermore, the chemical composition and/or phase of the electrolyte can modulate the surface charge transfer kinetics, leading to significant alterations in the spatiodynamics of lithium (de)insertion. In my talk, I will discuss how the liquid electrolyte-electrode interface controls the overall lithium (de)insertion pathway. Later, I will delve into how solid-electrolyte-electrode interfaces further complicate the entire process



Symposium : **KCS7-4**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 14:25

Chair: Jongwoo Lim (Seoul National University)

Crystallographic/electrochemical mechanism analysis of cathode materials for sodium-ion batteries

Munseok Chae

Nanotechnology Engineering, Pukyong National University, Korea

Various types of sodium manganese oxide show promise as host materials for sodium storage systems. One of the most significant advantages of this material family is their abundant nature. Among the various compositions, tunnel-type sodium manganese oxide stands out as a promising cathode for aqueous/nonaqueous sodium-ion batteries. However, its storage mechanism is not fully understood, partly due to the complex sodium intercalation process. Additionally, the limited cyclability caused by manganese dissolution has hindered its practical application in rechargeable batteries. In this study, we unveil the intricate sodium intercalation mechanism of tunnel-type sodium manganese oxide and propose a durable cathode surface film. The sodium storage mechanism of Na0.44MnO2 was meticulously characterized using a combination of electrochemical analysis, structure determination from powder XRD data, 3D bond valence maps, and energy calculations for sodium diffusion barriers. Furthermore, we report the discovery of a new P2-type Al/F-doped sodium manganese oxide, along with its unique sodium storage mechanism. This substitution significantly enhances the material's characteristics as a high-energy sodium-ion cathode. Al/F-doping provides structural stability through Jahn-Teller distortion and reduces the diffusion barrier due to their monovalency. Moreover, from a crystallographic perspective, the highly active P2-type ordering persists during long-term charge/discharge processes, avoiding inactivation caused by O3 transformation.

Symposium : **KCS7-5**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 14:50

Chair: Jongwoo Lim (Seoul National University)

Redox Flow Deionization (RFD): Principles, Progress, and Future Directions

Choonsoo Kim

Department of Environmental Engineering, Kongju National University, Korea

Recently, redox flow deionization (RFD) has received considerable attention in the field of water desalination as a promising electrochemical method for ion separation. The RFD configuration builds on the fundamentals of redox flow batteries by incorporating intermediate channels tailored for the passage of water streams. A unique feature of this system is the incorporation of multiple channels, which allows autonomous manipulation of different flow streams, such as the aqueous stream and the redox streams. This arrangement provides several advantages over conventional electrochemical ion separation techniques such as capacitive deionization and electrodialysis: 1) The sustained nature of the redox reactions allows cells to operate at low voltage levels, promoting versatility in the selection of electrode materials. 2) The mild reaction conditions minimize by-product formation and pH fluctuations. This facilitates downstream processes and improves system compatibility. 3) The energy stored in the redox couples facilitates an energy recovery process concurrent with ion separation, culminating in increased energy efficiency for water desalination efforts.In keeping with the trajectory of RFD advancement, the objective of this presentation is to introduce the fundamental principles underlying the RFD system as well as the recent advances made in its development. This includes an elucidation of the cell architecture, operating modes, and scale-up strategies. Furthermore, the discussion extends to various applications, such as the recovery of valuable resources and the management of pollutants. Finally, an overview of pragmatic challenges and potential avenues for future research exploration is presented.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS7-6**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 15:15

Chair: Jongwoo Lim (Seoul National University)

Digital Era in Chemistry Classes and Laboratories

Byeong-Seon Kim

Department of Chemistry Education, Gyeongsang National University, Korea

Digital transformation offers innovative methodologies and opportunities in modern scientific research. Organic chemistry laboratories can also benefit from digital transformation to enhance the efficiency and accuracy of experimental processes. This includes the utilization of advanced laboratory equipment and sensor networks for experiment data collection and management, as well as the application of artificial intelligence and machine learning for automated analysis. Additionally, the establishment of automation systems within the laboratory can streamline repetitive and time-consuming tasks. In this presentation, we will introduce the importance and advantages of digital transformation in organic chemistry laboratories, aiming to improve research efficiency and outcomes.

Symposium : **KCS7-7**
[KCS] Special Symposium for Young Chemists
Room 302+303 WED 15:40
Chair: Jongwoo Lim (Seoul National University)

A Study on the Reduction of H2 Boil-off of Liquefied Hydrogen for Long-Range Hydrogen Transportation

Hyunchul Oh

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

Liquefied hydrogen (LH2) is an energy source with a high volumetric energy density and is suitable for hydrogen transportation because it can reduce operating costs. However, due to the low evaporation temperature (20 K), phase changes (liquid to gas) inside the container cause considerable volume changes and evaporation losses, which in turn cause problems in long-term storage and transportation. For this reason, long-distance inland transport via tube trailers results in approximately 1- 15% (H2 boil-off) evaporation loss per day, depending on the volume. This presentation will discuss ways to reduce the boil-off loss of LH2 and enable long-distance transportation and long-term storage. It was speculated that the adsorption density of hydrogen adsorbed inside the porous material was similar to that of liquid hydrogen (70.8 kg/m3), but a recent study found that at 20 K, the adsorption density was higher than that of solid hydrogen (89.0 kg/m3). Therefore, using the porous adsorbent's physical adsorption method, it is expected that the loss of space due to dead volume can be supplemented with high-density adsorption hydrogen, and the hydrogen boiling point (20 K) can be increased to more than critical temperature (33.2 K). This study used a metal-organic skeleton (MOF) as a nanoporous material, and the degree of hydrogen boil-off was measured based on five samples (MOF-177, MFU-4l, DUT-6, MIL-53, and MOF-74) that have representative characteristics of MOF. As a result, the sample of DUT-6 showed about 96% storage performance compared to the amount of liquefied hydrogen theoretical storage, and the desorption temperature also increased to 35 K @ 1 Bar. These high-density hydrogen adsorption results were proved through neutron experiments and void volume calculations.

Symposium : **KCS7-8**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 16:15

Chair: Yunmi Lee (Kwangwoon University)

Elucidating DNA Damage and Repair in Cells, and Harnessing Them with In Situ Enzymatic Chemical Modification of DNA

Yong Woong Jun

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

The genetic information is continuously challenged by DNA-damaging events. DNA repair systems provide surveillance throughout our cells, maintaining the genomic integrity. Not surprisingly, deficiency in DNA repair activity which can arise from aging and genetic diseases is intimately linked to cancer, inflammation, and neurodegenerative diseases. However, monitoring DNA repair activity in the cellular context is challenging.We are interested in developing biochemical means to study DNA damage and repair processes in cells where all the essential components for DNA repair enzymes exist. Delineating DNA damaging pathways (and, of course, its repair responses) is of great interest to public health, as it is pivotal to find a way to reduce the accumulation of the damage in our genome. Our recent study shows that damaged DNA in cooked food might be an actual threat regarding the association of consuming cooked food at high temperatures with numerous health risks. We found that DNA in food gets damaged during the cooking process at high temperatures which finds its way to human genomic DNA upon consumption.DNA repair enzymes which are highly efficient and reliable can be harnessed with DNA modification by exploiting damaged DNA. We introduce in situ enzymatic chemical modification of DNA by simply mixing three components in a single tube–a DNA polymerase incorporating damaged nucleotides into DNA, a DNA repair excising the damage, and chemical compounds covalently binding to the resulting AP sites.

Symposium : **KCS7-9**
[KCS] Special Symposium for Young Chemists
Room 302+303 WED 16:40
Chair: Yunmi Lee (Kwangwoon University)

Supramolecular chemistry for functional two-dimensional materials

Yongju Kim

KU-KIST Graduate School of Converging Science and Technology, Korea University, Korea

Supramolecular chemistry based on non-covalent intermolecular interactions is an attractive tool for the sophisticated fabrication of various nanostructures. Among the various supramolecular structures, 2D sheet structures are interesting materials due to their extremely high surface area coupled with many unique chemical and physical properties, thereby offering the potential for new functional materials. In particular, the use of supramolecular 2D materials in biological applications can improve target molecule detection sensitivity, molecular loading, and bio-conjugation efficiency. Herein, I present functional supramolecular 2D materials that have a range of impressive applications. Synthetic aromatic amphiphiles are introduced as highly suitable building blocks for creating well-defined supramolecular 2D structures due to their rigid structure and π–π stacking of aromatic groups. These materials have been developed for chiral separations, vesicular transformations, myoblast stimulations, microbial agglutination regulations, and pH-responsive chiral inversions.

Symposium : **KCS7-10**

[KCS] Special Symposium for Young Chemists

Room 302+303 WED 17:05

Chair: Yunmi Lee (Kwangwoon University)

Water-Accelerated Sustainable and High-Turnover Organocatalysis for SuFEx Chemistry

Han Yong Bae

Department of Chemistry, Sungkyunkwan University, Korea

Amidst the growing demand for sustainable catalysis, the spotlight has turned toward the efficient synthesis and uncomplicated purification of complex organic molecules. In this presentation, we will discuss a compelling array of water-accelerated new organocatalytic transformations.First, N-heterocyclic carbene (NHC)-catalyzed aza-Michael addition reaction will be shown, offering simple access to β-aminosulfonyl fluorides. These compounds are pivotal hubs for the sulfur(VI) fluoride exchange (SuFEx) click chemistry.[2] In addition, novel methodologies leveraging high-turnover catalytic Michael and thia-Michael additions, amplified through significant hydrophobic interactions, will be unveiled. A synergistic action of hydrophobic Brønsted acid in combination with a hydrogen-bonding donor activator will be disclosed: this innovative combination orchestrates the three-component Petasis-type allylation reaction. The catalytic systems devised exhibit remarkable mildness and potency, accommodating a wide array of substrates and facilitating efficient multi-gram scalability. The incorporation of water remarkably accelerates the reaction rates while upholding exceptional chemo- and site-selectivity (up to >99:1), surpassing the performance of conventional organic solvents.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS7-11**
[KCS] Special Symposium for Young Chemists
Room 302+303 WED 17:30
Chair: Yunmi Lee (Kwangwoon University)

Harnessing Innate Immune Modulators for Therapeutic Innovation

Hyejin Kim

Infectious Diseases Therapeutic Research Center, Korea Research Institute of Chemical Technology, Korea

The field of innate immune modulation offers exceptional prospects in both immuno-oncology and vaccine development. Recent breakthroughs highlighting the potential of activating innate immunity for bolstering immunotherapeutic effects have spurred dedicated efforts to apply this approach to anticancer interventions. Simultaneously, recognizing the pivotal role of immunity in vaccination, researchers are actively exploring the integration of innate immune activation as adjuvants to amplify vaccine responses.This presentation aims to spotlight significant protein targets within the innate immune system, unveiling their crucial roles. We developed activator molecules designed to enhance the functionality of these targets. The results find applications in immuno-oncology, where activating these targets enhances the efficacy of cancer immunotherapies, as well as in vaccines, promising to revolutionize adjuvant strategies and bolster vaccine potency. This abstract focuses on the role of STING agonists in fortifying anticancer immune responses and their potential as immune checkpoint modulators. Simultaneously, it highlights the progress in utilizing TLR7/8 agonists as potent vaccine adjuvants. These strategies bear the promise of reshaping therapeutic landscapes, enhancing immunotherapy and vaccination strategies, ultimately leading to improved patient outcomes.

Symposium : **KCS8-1**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 14:00

Chair: Yongwon Jung (KAIST)

Statistical Thermodynamics and Chemical Dynamics of Nucleus Seed Formation and Ensuing Phase Transitions in Complex Biological and Material Systems

Jaeyoung Sung

Creative Research Initiative Center for Chemical Dynamics in Living Cells and Department of Chemistry, Chung-Ang University, Korea

We briefly introduce our generalization of the continuous-time random walk model and renewal theory, which is useful for quantitative investigations into the transport dynamics and reaction dynamics of complex biological or material systems [1,2] We will then focus on our recent work on statistical thermodynamics and chemical dynamics of nuclei seed formation and ensuing phase transitions dependent on experimental conditions. This work sheds light on the thermodynamic origin of monodisperse nuclei seed formation and provides a unified, quantitative explanation for not only the time-dependent size distribution but also the size-dependent growth dynamics of nanoparticle systems, which cannot be explained by the classical nucleation theory or any previous theories of nucleation.

References:

[1] Song et al., Transport Dynamics in Complex Fluids, Proc. Nat. Acad. Scie. U.S.A. 116, 12733 (2019); Poletayev et al., Defect-driven anomalous transport in fast-ion conducting solid electrolytes, Nat. Mater. 21, 1066 (2022). Kang et al., Real-space imaging of nanoparticle transport and interaction dynamics by graphene liquid cell TEM, Sci. Adv. 7, 49 (2021).

[2] Kang et al, Stochastic kinetics of nanocatalytic systems, Phys. Rev. Letters 126, 126001 (2021); Park et al., The Chemical Fluctuation Theorem governing gene expression, Nat. Commun. 9, 297 (2018); Lim

et al., Quantitative understanding of probabilistic behavior of living cells operated by vibrant reaction networks, Phys. Rev. X 5, 031014 (2015).

Symposium : **KCS8-2**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 14:25

Chair: Yongwon Jung (KAIST)

The organization and function of biomolecular condensates centered around RNA

Yongdae Shin

Seoul National University, Korea

Phase separation involving biomolecular liquids is emerging as a fundamental mechanism of intracellular organization. Multiple distinct condensates coexist within cellular space to compartmentalize biomolecules and facilitate the flow of genetic information. In this talk, I will discuss our recent efforts to study the organization and function of biomolecular condensates with a particular focus on RNA. Combining an optogenetic tool for the control of intracellular phase separation with single-molecule RNA imaging, we monitor the dynamics and activity of RNA molecules localized to condensates. We find that sequestering RNA leads to the inhibition of translation activity, in a manner dependent on the material properties of condensates. I will also discuss the role of RNA in regulating the density of condensates. Together, our work highlights the tight interplay between RNA and condensate properties.

Symposium : **KCS8-3**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 14:50

Chair: Yongwon Jung (KAIST)

Network Structure and Dynamics of Biomolecular Condensates

Jeong-Mo Choi

Department of Chemistry, Pusan National University, Korea

There is growing interest in uncovering the fundamental principles of liquid-liquid phase separation (LLPS) of multivalent proteins with intrinsically disordered regions, given the direct relevance to the reversible formation/dissolution of biomolecular condensates. However, despite recent advances in the field, achieving multiscale structural characterization of these liquid condensates remains an outstanding challenge. Nucleophosmin (NPM1) stands out as a key component of the liquid-like granular component (GC) within the nucleolus. To gain insight into these systems, a minimal model of NPM1, designated as N130, has been developed. This minimal model, N130, encompasses the N-terminal fragment of NPM1, retaining two acidic tracts and the ability to oligomerize into homopentamers. Notably, N130 has the capacity to induce LLPS in the presence of arginine-rich (R-rich) peptides.In this presentation, I will discuss our recent investigation on phase separation involving various combinations of N130 and R-rich peptides. Our study aimed to decipher the structural nuances of the resulting phase-separated condensates, employing small-angle neutron scattering (SANS) measurements. Additionally, we employed theoretical models and multiscale computer simulations to unveil the intricate molecular characteristics underlying the experimental structural profiles. Collectively, these experimental and theoretical insights not only contribute to our current understanding but also pave the way for a quantitative comprehension of the liquid-like attributes within the NPM1-rich GC region of the nucleolus in the future.

Symposium : **KCS8-4**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 15:15

Chair: Yongwon Jung (KAIST)

Microdroplet Chemistry: Chemical Reactions at Heterogenous Phase Interfaces

Jae Kyoo Lee

Applied Bioengineering, Seoul National University, Korea

This talk will present microdroplet chemistry, the studies of unusual properties of chemical reactions in and at the interfaces of microdroplets. We found that chemistry in liquid microdroplets, which can mediate the transition from the solution to the gas phase reactions, markedly differs from those in solution and gas phases. These unique properties include the acceleration of reaction rates, thermodynamic changes, self-assembly of nanostructures, and spontaneous charge exchange. Various chemical reactions, including protein unfolding, redox reactions, hydrogen-deuterium exchange, and crystallization, are accelerated by over a factor of a thousand in microdroplets. Besides, the thermodynamics of chemical reactions are also altered in water microdroplets. We found that molecules are in highly ordered states near the microdroplet interface. This lowered entropic barrier allows thermodynamically unfavorable reactions, such as phosphorylation and RNA formation, to proceed without any enzyme or ATP energy source at room temperature in water microdroplets. Moreover, the charge exchange between water and solute molecules spontaneously occurs at the water interface, leading to the oxidation of water molecules and the reduction of solute molecules. Liquid-liquid phase separation in aqueous solution induces the formation of microdroplets in cells, called cellular condensates. This talk will also describe the chemical reactions at the cellular condensate interface and the application of microdroplet chemistry to various energy, environmental, and biomedical research fields.

Symposium : **KCS8-5**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 16:00

Chair: Jeong-Mo Choi (Pusan National University)

Kinetics of Protein Phase Transitions

Tuomas Knowles

Yusuf Hamied Department of Chemistry, University of Cambridge, United Kingdom

Proteins are able to access a number of different states, some connected with biological function and others associated with malfunction. This talk explores experimental and theoretical analysis of the rates at which proteins can undergo such transitions, focusing on the liquid condensate and solid amyloid phase of proteins. We will discuss a number of examples where the study of kinetics gives insights into the fundamental molecular mechanisms that underlie protein phase transitions. Many of these mechanisms draw on soft condensed matter concepts and phenomena. Condensate modulation will be discussed both from the point of view of understanding fundamental biological function as well as ameliorating malfunction in the context of the onset and development of neurodegenerative diseases.

Symposium : **KCS8-6**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 16:35

Chair: Jeong-Mo Choi (Pusan National University)

Molecular basis for SOX2-dependent regulation of super-enhancer activity

Kyeong Kyu Kim

Department of Medicine, Sungkyunkwan University, Korea

Pioneer transcription factors (TFs) like SOX2 are vital for stemness and cancer through enhancing gene expression within transcriptional condensates formed with coactivators, RNAs, and mediators on super-enhancers (SEs). Despite their importance, how these factors work together for transcriptional condensation and activation remains unclear. SOX2, a pioneer TF found in SEs of pluripotent and cancer stem cells, initiates SE-mediated transcription by binding to nucleosomes, though the mechanism isn't fully understood. To address SOX2's role in SEs, we identified mSE078 as a model SOX2-enriched SE and p300 as a coactivator through bioinformatic analysis. In vitro and cell assays showed SOX2 forms condensates with p300 and SOX2-binding motifs in mSE078. We further proved that SOX2 condensation is highly correlated with mSE078's enhancer activity in cells. Moreover, we successfully demonstrated that p300 not only elevated transcriptional activity but also triggered chromatin acetylation via its direct interaction with SOX2 within these transcriptional condensates. Finally, our validation of SOX2-enriched SEs showcased their contribution to target gene expression in both stem cells and cancer cells. In its entirety, this study imparts valuable mechanistic insights into the collaborative interplay of SOX2 and its coactivator p300, shedding light on the regulation of transcriptional condensation and activation within SOX2-enriched SEs

Symposium : **KCS8-7**

[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors

Room 304+305+306 WED 17:00

Chair: Jeong-Mo Choi (Pusan National University)

Phase Transitions of Confined Water at the Nanoscale

Joonkyung Jang

Department of Nanoenergy Engineering, Pusan National University, Korea

Using Monte Carlo (MC), molecular dynamics (MD) simulations and theory, we examined the phase behavior of confined water for two representative systems which are important in surface science and nanotechnology. First, we study the (de)wetting transition of water confined between an atomic force microscope (AFM) tip and the underlying surface. We investigate the liquid-to-vapor phase transition of the confined water as the AFM tip approaches the surface. By projecting the density of states (DOS) of water into the liquid-like and solid-like contributions, we reveal the energetic and entropic contributions in the (de)wetting transition. Implications of these results for interpreting an AFM measurement are discussed. Second, we study the phase behavior of the interfacial water contacting a surface corrugated with the nanoscale grooves. A continuum theory is developed for the critical inter-pillar spacing which induces the wetting transition of the grooves. We also present a theory for the free energy profile with respect to the level of liquid filling into the grooves. Using MC and MD simulations, we uncover various intermediate states in the continuous wetting of the grooves, including the (meta) stable and transition states and activation energies.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS8-8**
[Chemistry Symposium for Future Innovation] Convergent Understanding of Phase Transition Behaviors
Room 304+305+306 WED 17:25
Chair: Jeong-Mo Choi (Pusan National University)

Protein models to study biomolecular phase separation

Yongwon Jung

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

Phase separation of specific biomolecules into liquid droplet-like condensates (process called liquid-liquid phase separation, LLPS) is a key mechanism to form membrane-less organelles, which spatio-temporally organize diverse biochemical processes in cells. For more clear and precise analysis of these condensates, it is critical to have diverse but simplified model systems. Our group have developed various protein-based in vitro LLPS models to elucidate distinct behaviors of biomolecular membrane-less organelles. These models include metal ion-induced clustering of minimal protein modules and clustered intrinsically disordered proteins (IDPs) or light-controllable IDPs. In this talk, several examples of LLPS model-based investigation of molecular and structural codes of droplet-forming proteins will be discussed. In addition, our recently developed strategy to monitor nucleation in real time during protein phase separation will also be introduced.

Symposium : **KCS9-1**

[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science

Multipurpose Hall 1 FRI 10:15

Chair: Natalie Stingelin (Georgia Institute of Technology)

Tailoring the Photophysics of First-row Transition Metal-based Chromophores for Applications in Light-to-Chemical Energy Conversion: Challenges and Opportunities

James K. McCusker

Department of Chemistry, Michigan State University, United States

The conversion of light to chemical energy is one of the most fundamental processes on Earth. Research on solar energy conversion has sought to replicate Nature's solution through the realization of artificial constructs that mimic various aspects of photosynthesis. The critical first step in this process is the absorption of light and subsequent separation of charge. Transition metal-based chromophores are particularly well-suited for use in such schemes by virtue of the charge-transfer excited-states that a majority possess. Indeed, tremendous advances have been made through use of compounds such as $[\mathrm{Ru(bpy)}^{3}]^{2}$+, but despite their obvious advantages the fact that these compounds are built upon elements that are among the rarest in the earth's crust raises legitimate questions concerning cost and scalability of processes reliant on such chromophores. Coupled with the possibility of unlocking new chemistry, this circumstance has motivated efforts to replace these compounds with chromophores based on earth-abundant first-row transition metals that can carry out analogous excited-state reaction chemistry. With these opportunities come significant challenges due to inherent differences in the electronic structures of first- versus second- and third-row metal complexes that profoundly impact the ability of such compounds to engage in the desired chemistry. This seminar will focus on our efforts – encompassing synthesis, spectroscopy, and theory – to understand the factors that determine the dynamics associated with the excited states of first-row transition metal-based chromophores with the ultimate goal of circumventing and/or redefining their intrinsic photophysics in order to make feasible their use in a variety of light-driven applications.

Symposium : **KCS9-2**

[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science

Multipurpose Hall 1 FRI 10:45

Chair: Natalie Stingelin (Georgia Institute of Technology)

Accelerated chemical science using AI

Yousung Jung

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

Discovery of new molecules and materials with desired properties is a practical goal of chemical research. A promising way to significantly accelerate the latter process is to incorporate all available knowledge and data to plan the synthesis of the next materials. In this talk, I will present several directions to use informatics and machine learning to efficiently explore chemical space. I will first describe methods of machine learning for fast and reliable predictions of materials and molecular properties. With these tools in place for property evaluation, I will then present a few generative frameworks that we have recently developed to allow the inverse design of molecules and materials with optimal target properties, either in the compositional space or structural space. One general challenge in digital discovery is that many of the molecules and materials that are computationally designed are often discarded in the laboratories since they are not synthesizable. I will thus lastly spend some time to talk about the synthesizability of molecules and materials, either by predicting the synthesis pathways (retrosynthesis) or chemical reactivity. Several challenges and opportunities that lie ahead for further developments of accelerated chemical platform will be discussed.

Symposium : **KCS9-3**

[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science

Multipurpose Hall 1 FRI 11:15

Chair: Natalie Stingelin (Georgia Institute of Technology)

Excited state trajectories in photoactive transition metal complexes probed by ultrafast laser and x-ray spectroscopies and scattering

Lin X. Chen

Northwestern University, Argonne National Laboratory, United States

Many photochemical events start from initial light-matter interactions that cause atomic and electronic displacements in the excited states away from the energy minima of their potential energy surfaces. When certain photochemical events, such as bond breaking, intersystem crossing and electron/energy transfer taking place within the periods of key vibrational modes, the excited state energies are determined by the trajectories defined by the actual nuclear movements that may lead to different reaction pathways and outcome. Examples will be given in the work of tracking excited state pathways for transition metal complexes on the time scales from femtosecond to a few picoseconds, such as excited state Cu(I) and Pt(II) dimer complexes. Using fs broadband transient spectroscopy and fs X-ray solution scattering, coherent vibrational wavepacket motions can be examined.

From the time evolution of key vibrational modes in the Pt dimer complexes, particularly the Pt-Pt stretching mode, we mapped out excited state trajectories on potential energy surfaces of Pt-dimer complexes for light conversion, including coherent nuclear motions. These studies were carried out in a series of model platinum dimer complexes in solution and their electron donor acceptor complexes, featuring rich photochemistry and a set of intricate excited state potential energy surfaces on time scale previously unattainable.

(Optional) For the time evolution of the structural dynamics of Cu(I) complex, the experimental results revealed the Jahn-Teller distortion that transforms the symmetry of the molecule from the D2d in the ground state to D2 in the triplet metal-to-ligand-charge-transfer (MLCT) state along the two key cooperative coordinates, the Cu-N distances and the angle between the two phenanthroline ligand planes.

The detailed structural trajectories have been reproduced by quantum mechanical calculations to map out the actual excited state nuclear motions from the Frank-Condon structure to an intermediate triplet state and finally the triplet MLCT state.

Symposium : **KCS9-4**
[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science
Multipurpose Hall 1 FRI 11:45
Chair: Natalie Stingelin (Georgia Institute of Technology)

Facile methods for engineering performance improvements in perovskite photovoltaics

Martyn A. McLachlan

Department of Materials, Imperial College London, Molecular Sciences Research Hub, Wood Lane, London, United Kingdom

Metal halide perovskites (MHPs) continue to stimulate interest, generate significant research volume, and fuel scientific discussion and debate. The rapid evolution and deployment of MHPs to the commercial realm has been a remarkable journey. These materials, and their precursors, afford numerous synthetic pathways from a plethora of starting materials via a variety of processes – the sum of which are complex, multi component functional materials around which numerous scientific questions remain unanswered. Here we investigate the role of additives and post-deposition processing and their influence of morphology and microstructure on photovoltaic device performance and MHP stability.

Many strategies have emerged for tuning the properties of MHPs from substitutional doping to influence bandgap and electronic properties to additive incorporation to tune lifetime and stability – collectively resulting in a diverse range of compositions or “flavours” of MHPs being reported. Here I will discuss strategies reliant on additive incorporation that result in improvements in photovoltaic device performance and stability. In parallel we consider the interaction such additive molecules have with the MHP films and by utilising a range of correlative characterisation techniques we probe the location where our additives reside and the influence they have on the microstructure and morphology. By carrying out systematic studies of isolated MHP films, films sandwiched with interlayers and complete devices we explain the key relationships between structure, composition and performance of our additive engineered perovskite solar cells.

Symposium : **KCS9-5**

[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science

Multipurpose Hall 1 FRI 14:30

Chair: Seong-Ju Hwang (Yonsei University)

Deciphering structure/property interrelations for functional polymer systems using thermal analysis

Natalie Stingelin

School of Materials Science & Engineering, Georgia Institute of Technology, United States

In recent years, immense efforts in the functional polymer field have led to unprecedented progress and to numerous new opportunities for polymers in, e.g., electronics, energy storage, energy harvesting, health care, and beyond. Despite these advances, many challenges still exist: predicting properties, identifying reliable processing protocols and, more fundamentally, gaining a complete understanding of the way structural features over all length scales affect functions in macromolecular matter, including electron/ion transport, charge generation, ferroelectric characteristics, and/or photophysical processes. Here we demonstrate how classical polymer science tools can be used to elucidate the structure development of functional polymers from the liquid phase, how such knowledge can be exploited to manipulate their phase transformations and solid-state order and, in turn, their performance. We provide examples how side-chain softening can influence mechanical and optoelectronic properties, and how vitrification can dominate the structure formation of ferroelectric:semiconducting polymer blends. We moreover discuss how differential scanning calorimetry techniques, including fast calorimetry, can be used for the identification of thermodynamic transitions of "unusual" polymers, including ribbon-like polymers (used, e.g., in organic solar cells) or high-refractive index inorganic:organic hybrid materials. Generally, we will demonstrate how thermal analysis can be exploited to obtain important structural information of these new material classes and, in turn, how processing guidelines can be established towards materials of specific optical or electrical characteristics, towards improved materials design and new understanding of this next generation polymer systems

Symposium : **KCS9-6**

[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science

Multipurpose Hall 1 FRI 15:00

Chair: Seong-Ju Hwang (Yonsei University)

Understanding catalyst-electrolyte interfaces for electrochemical CO_2 conversion

Yun Jeong Hwang*, **Suhwan Yoo**

Department of Chemistry, Seoul National University, Korea

Electrochemical CO_2 reduction (CO_2R) can be integrated with renewable energy sources and water can be utilized as a direct proton source which is promising to provide a sustainable net-zero carbon cycle. However, controlling undesired competitive hydrogen evolution reaction (HER) from water electrolysis is crucial for selective CO_2R. Various metal-based electrocatalysts have been investigated to convert CO_2 to CO, formate, ethylene, ethanol, or other C_{2+} chemicals. Recent efforts to understand the electrocatalytic activity have found that the cations in the electrolyte play an important role to modulate the activity even for a given electrocatalyst. Therefore, the interface between the catalyst and electrolyte has to be carefully investigated. The relationship between the product distribution of CO_2R and its intermediate species can be monitored by operando spectroscopy studies. We demonstrate that *CO, one of the crucial intermediate, can be observed by Raman or Infra-red spectroscopy, and their vibrational wavenumbers depend on the electrolyte condition. Meanwhile, for a practical point of view, researchers also propose direct conversion of the captured CO_2 by electrochemical process. We demonstrate that a Ni-N-C catalyst has high selectivity for electrochemical CO_2 conversion to CO production due to the relatively high activation energy for HER compared to that of CO_2R-to-CO reaction. In addition, the Ni-N-C was found to have low sensitivity to the type of alkali metal cation or the type of amine. Modulation of the catalyst-electrolyte interface can provide new opportunities to promote challenging catalytic reactions.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **KCS9-7**
[KCS-RSC Joint Symposium] Multidisciplinary Approach to Energy Science
Multipurpose Hall 1 FRI 16:00
Chair: Seong-Ju Hwang (Yonsei University)

Publishing with the RSC

Michaela Muehlberg

Executive Editor of Journal of Materials Chemistry A B & C, Royal Society of Chemistry, United Kingdom

An introduction to the Royal Society of Chemistry and its activities followed by a short overview of the RSC's materials journals, a quick guide on the publishing process and what to be aware of when writing your research article.

Symposium : **POLY1-1**
Recent Trends in Polymer Synthesis
Room 302+303 THU 15:40
Chair: In-Hwan Lee (Ajou University)

Transition-Metal Catalysis for Sustainable Polymer Synthesis

Hye-Young Jang

Department of Chemistry, Ajou University, Korea

The urgent need to address global warming and environmental concerns has prompted the exploration of sustainable carbon resources, thereby shifting focus away from fossil fuels. In line with this, it becomes imperative to replace commercially important polymer production that relies on petroleum resources with more sustainable alternatives. In this presentation, we would like to show the metal-catalyzed polymerizations that employ CO2 to produce polycarbonate-polyol and glycidol for polyglycerol synthesis. Both reactants used in these polymerizations are considered sustainable resources; CO2, a well-known greenhouse gas contributing to global warming, can be captured and utilized, and glycidol is derived from biodiesel byproducts. The synthesis of polycarbonate-polyol, we employed Zn-based double-metal cyanide catalysts. The catalytic activity of DMC catalysts was notably enhanced by using morphology-controlled Zn-glutarate. On the other hand, copper complexes coordinated with tri-N-heterocyclic carbene (triNHC) were used to catalyze the polymerization of glycidol. A key feature of this process is the remarkably low degree of branching (DB) observed in the resulting polyglycerol. The unique structure of Cu(triNHC) played a key role in inducing low DBs in polyglycerol. In this presentation, we will provide polymerization results as well as the characterization of polymers and catalysts involved in both processes. By adopting these sustainable approaches, we aim to pave the way for eco-friendly polymer production.

Symposium : **POLY1-2**
Recent Trends in Polymer Synthesis
Room 302+303 THU 16:05
Chair: In-Hwan Lee (Ajou University)

Design of Topology-Controlled Polyethers toward Robust Cooperative Hydrogen Bonding

Sang-Ho Lee

Korea Research Institute of Chemical Technology, Korea

As a function of important molecular parameters, controlling the polymer topologies is critical to determine the physical properties and applications. Particularly, the polymer topologies, carrying numerous hydrogen bonding (H-bonding) donor and acceptor in polymer chains, strongly influence their unique properties by inducing the different inter- and intramolecular H-bonding. Herein, we present the investigation of a high-level control of the inter- and intramolecular H-bonding in the topology-controlled poly(glycidoxy carbonyl benzoic acid)s (PGCs) (i.e., linear, hyperbranched, and branched cyclic structures having a similar degree of polymerization). The topology-controlled PGCs were successfully prepared by introducing the aromatic carboxylic acids in the corresponding polyglycidols (PGs) via quantitative post-polymerization modification using phthalic anhydride and organic base as a nucleophilic catalyst. The resulting polymers were analyzed by 1H NMR, SEC, and TGA. The obtained three types of PGCs were demonstrated the high-level interplay between the inter- and intramolecular H-bonding in polymer chains by exhibiting the pH-dependent self-association properties in the solution state and the strong adhesion properties in the bulk state with high transparency. Interestingly, the dramatically enhanced adhesive property by 2.6-fold was demonstrated by simple mixing of branched cyclic PGC and topology-controlled PGs to promote the cooperative H-bonding between polymer chains. We anticipate the new class of cooperative H-bonding between topology-controlled polymers contribute to the development of advanced adhesive and the high potential in biological and biomedical applications due to its excellent biocompatibility.

Symposium : **POLY1-3**

Recent Trends in Polymer Synthesis

Room 302+303 THU 16:40

Chair: In-Hwan Lee (Ajou University)

Synthesis of well-defined polymers containing triphenylamine group via living anionic polymerization for hole-transporting layer of solution-processable organic light-emitting diodes

Beom-Goo Kang

Department of Chemical Engineering, Soongsil University, Korea

Anionic polymerization is the most well-established living polymerization system and is used to prepare well-defined polymers with predictable molecular weights and narrow molecular weight distributions. Among various functional groups, particular emphasis has been placed on triphenylamine. This functional group garners significant interest for its application in organic electronic devices, including organic light-emitting diodes (OLEDs), photovoltaics, and resistive memory owing to its hole-transporting properties. The forthcoming presentation will mainly focus on the precise synthesis of homopolymer and block copolymer containing triphenylamine group via living anionic polymerization. Furthermore, we will discuss their solvent orthogonality and potential application as hole-transporting layer in solution-processable OLEDs.

Symposium : **POLY1-4**

Recent Trends in Polymer Synthesis

Room 302+303 THU 17:05

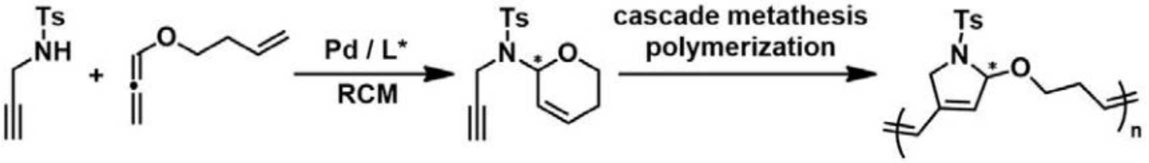
Chair: In-Hwan Lee (Ajou University)

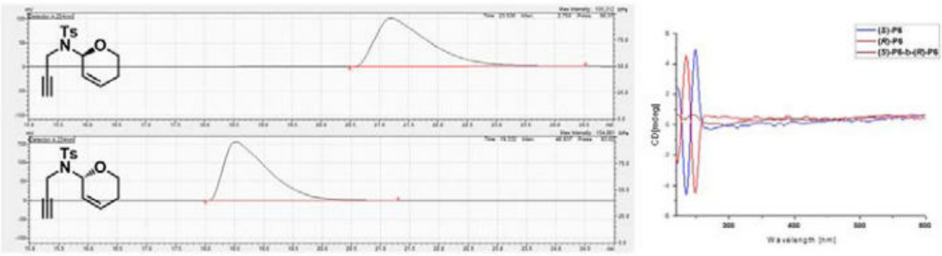
Living cascade enyne metathesis polymerization for stereo-defined degradable polymer and its application in controlling the molecular weight distribution

Cheoljae Kim

Department of Chemistry, Chungbuk National University, Korea

We have developed a degradable polymer from N,O-acetal containing enyne monomer via cascade enyne metathesis polymerization. Enynes were obtained with high optical purities through Pd-catalyzed asymmetric hydroamination of alkoxyallenes from propargyl amines, followed by ring-closing metathesis of the generated dienyne. With the living characteristics of polymerization, copolymers were obtained by controlled addition of the corresponding monomers such as stereo-controlled blocks as well as degradable and non-degradable blocks. Additionally, the control of monomer feeding provided various molecular weight distributions of the obtained polymers.





Award Lecture in Division : **POLY2-4**
Special Symposium by Mid-Career Polymer Chemists
Room 302+303 FRI 10:25
Chair: Myungeun Seo (KAIST)

Universal 3D Crosslinkers for All-Solution Processed Electronics

BongSoo Kim[*], MyeongJae Lee[1]

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

We present the all-solution processing of highly integrated arrays of organic thin-film transistors, organic light-emitting diodes, and quantum-dot light-emitting diodes. This processing is performed using newly developed multi-bridge photo-crosslinkers containing 4 or 6 photo-crosslinkable units. Under UV, photo-crosslinkers mixed within solution-processable electronic materials generate a three-dimensional (3D) network of the given host electronic materials. The 3D network state can be formed efficiently even at an unprecedentedly small loading (only 1 or lower wt%), without sacrifice of the intrinsic electrical properties of the host material. Also, the crosslinking of electronic component layers allows not only micropatterning of the layers at high resolution (< 5 μm) but also stacking of a given electronic component layer on top of the other layers.[1-3] Furthermore, our efficient photo-crosslinkers enable to produce an ultrathin polymer gate dielectric, the application of which results in excellent hole and electron mobilities of 12.4 and 10.1 cm2 V-1s-1, respectively, from p- and n-type OTFTs operated at < 3 V.[4] These works demonstrate that the use of photo-crosslinkers paves a new avenue to fabricate future electronic devices.References[1] "Universal Three-Dimensional Crosslinker for All-Photopatterned Electronics" Nat. Commun. 2020, 11, 1520.[2] "Tetrabranched Photo-Crosslinker Enables Micrometer-Scale Patterning of Light-Emitting Super Yellow for High-Resolution OLEDs" ACS Photonics 2021, 8, 2519.[3] “Nondestructive Photopatterning of Heavy-Metal-Free Quantum Dots” Adv. Mater. 2022, 2205504[4] “Low Voltage Organic Transistors Using Six-Branched Organic Azide” Chem. Mater. 2022, 33, 10409.

Symposium : **POLY2-1**

Special Symposium by Mid-Career Polymer Chemists

Room 302+303 FRI 09:00

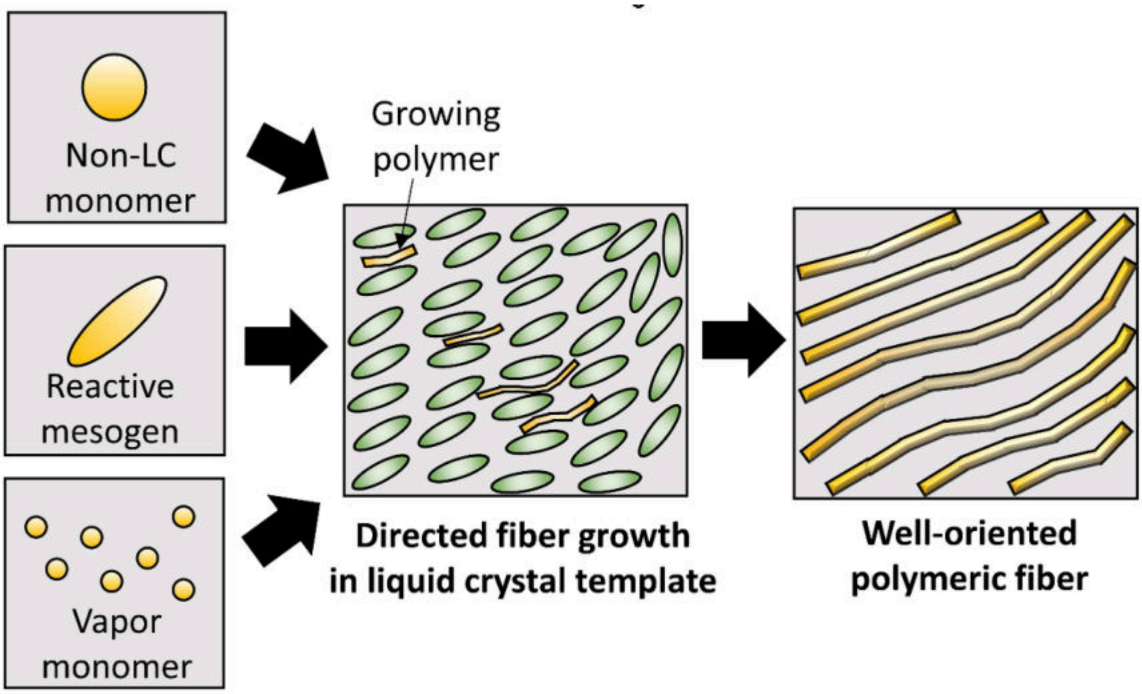
Chair: Myungeun Seo (KAIST)

Controlled Mesoscopic Growth of Polymeric Fibers Using Liquid Crystal Template

Dong Ki Yoon

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

Orientation-controlled polymeric fiber is one of the most exciting research topics to rationalize the multi-functionality for various applications. In order to realize this goal, the growth of polymeric fibers should be controlled using various techniques like extrusion, molding, drawing, and self-assembly. Among the various candidates to fabricate the orientation-controlled polymeric fibers, the template-assisted assembly guided by a liquid crystal (LC) matrix is the most promising because the template can be manipulated easily with various methods like surface anchoring, rubbing, geometric confinement, and electric field. This review introduces the recent progress toward the directed growth of polymeric fibers using the LC template. Three representative LC-templated polymerization techniques to fabricate fibers include chemical or physical polymerization from the monomers mixed in LC matrix, patterned fibers formed from LC-templated reactive mesogens, and orientation-controlled nanofibers by infiltrating vaporized monomers between LC molecules. The orientation-controlled polymeric fibers will be used in electro-optical switching tools, tunable hydrophilic or hydrophobic surfaces, and control of phosphorescence, which can open a way to design, fabricate, and modulate nano- to micron-scale fibers with various functions on demand.


Non-LC monomer
Reactive mesogen
Vapor monomer
Growing polymer
Directed fiber growth in liquid crystal template
Well-oriented polymeric fiber

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **POLY2-2**
Special Symposium by Mid-Career Polymer Chemists
Room 302+303 FRI 09:25
Chair: Myungeun Seo (KAIST)

Unconventional Low-voltage Organic Electronics Based on Electrochemical Doping/Dedoping and Their Application to Neuromorphic Devices

Myung-Han Yoon

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

In this research, we report unconventional low-voltage organic electronics based on lateral-type organic electrochemical diodes (OECDs) using organic mixed ionic-electronic conductors. The underlying mechanism on polarity-sensitive balanced ionic doping/dedoping is verified by numerical device simulation/analysis and in operando spectroelectrochemical potential mapping, while the general material requirements for electrochemical diode operation are deduced from various types of conjugated polymers. In parallel, analog signal rectification and digital logic processing circuits are successfully demonstrated to show the broad impact of circuits incorporating organic electrochemical diodes. Finally, two-terminal neuromorphic devices and their circuits are successfully fabricated by wiring multiple electrochemical diodes in parallel and/or in series.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **POLY2-3**
Special Symposium by Mid-Career Polymer Chemists
Room 302+303 FRI 10:00
Chair: Myungeun Seo (KAIST)

Porphyrin-based supramolecular polymers

Woo-Dong Jang

Department of Chemistry, Yonsei University, Korea

Porphyrins are essential pigments in biological systems. Porphyrins and chlorophylls are often self-assembled into nanoscale superstructures to perform many essential functions, such as light harvesting and electron transport. The crystal structure of the light-harvesting antenna complexes (LHC) in purple photosynthetic bacteria shows the presence of a highly symmetric wheel-like supramolecular architecture involving a large number of bacteriochlorophyll pigments. From the inspiration of the natural light-harvesting systems, a variety of porphyrin-based nanoarchitectures, such as nanofibers, nanosheets, nanoparticles, and nanorings have been fabricated for applications in various research fields including photonics, catalysis, and electronics. The mimicry of the light-harvesting system is a very important subject, not only from a scientific viewpoint but also for its possible contribution to the sustainable utilization of energy resources. As a mimic of a natural light-harvesting system, we recently have designed several porphyrin-based artificial models including porphyrin dendrimers, self-assembled nano-ring, and supramolecular receptors. In this symposium, we are going to report recent advances in our research related to porphyrin-based supramolecular polymers. For example, a porphyrin dyad containing a diacetylene bridge showed the formation of globular-shaped nanoparticles or linear fibrous supramolecular polymers depending on central metal ions. These results could pave the way for mimicking biological systems where the macroscopic hierarchical assemblies arise in response to the microscopic changes of biomolecules.

Symposium : **POLY3-1**
Recent Advances in Sustainable Polymer Materials
Room 302+303 FRI 14:30
Chair: Jeyoung Park (Sogang University)

Synthesis and Characterizations of Biomass Lignin-based Degradable Polymers

Hoyong Chung[*], Arijit Ghorai, Sundol Kim, Christian Gonzales, Lily Masa

Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Florida State University, United States

Lignin is the second most abundant renewable biomass polymer. Despite its potential as a sustainable raw material due to its abundance, low price, and high aromatic concentration, its complex structure and poorly defined excessive reaction sites for lignin limit its application. Castor oil is a type of triacylglycerol that consists of various fatty acids and glycerol. Especially, castor oil's hydroxyl group is very useful for further chemical modification. In this work, we have synthesized a 100% biomass-based polyester, lignin-graft-castor oil. The lignin was chemically modified by succinic acid and capping agent, acetic acid. Acetic acid capped the hydroxyl group to reduce the number of excessive reaction sites in the lignin, and succinic acid is used to introduce carboxylic acid for graft copolymerization to castor oil’s hydroxyl group. The castor oil was used in its pristine form without any modification. These two biomasses are covalently linked via carbodiimide mediated esterification. The synthesized lignin-graft-castor oil was thermoplastic demonstrating decent melting temperatures (57~71 oC) and glass transition temperatures (39~60 oC). The mechanical properties of new capped lignin-graft-castor oil can be controlled by changing the crosslinking density and the mass ratio of lignin and castor oil. The highest modulus is 228.43 MPa, which is higher than that of low-density polyethylene (LDPE). Furthermore, its physical properties, including density and contact angle of water, are also changed by the mol % of the capping agent and the mass ratio of lignin and castor oil. The new synthesized 100% biomass-based polymer, lignin-graft-castor oil, will be a new class of completely degradable polymer that will solve the non-degradable polymer waste issue.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **POLY3-2**

Recent Advances in Sustainable Polymer Materials

Room 302+303 FRI 14:55

Chair: Jeyoung Park (Sogang University)

Development of Adhesive for Laminated Electrical Steels Having Excellent Adhesion and Oil Resistance and Its Application for Dot-bonded Motor Core for Electric Vehicle

Ki-Tae Kang

Samyang Corporation, Korea

Herein we prepared an adhesive for laminated electrical steels that has excellent adhesion and oil resistance for dot-bonded motor core for electric vehicles. Its outstanding adhesion and oil resistance originate from isosorbide core structure having good hydrophilicity and a rigid chemical structure. The adhesion property was evaluated by measuring the lap shear strength of the laminated electrical steel and peel strength of the dot-bonded motor core and compared it to an adhesive to which petroleum-based alicyclic polyol was applied. Isosorbide derivative was incorporated in acrylate modified polyurethane as a polyol for compatibility with other adhesive components and to enact a fast-curing process.

Symposium : **POLY3-3**

Recent Advances in Sustainable Polymer Materials

Room 302+303 FRI 15:30

Chair: Jeyoung Park (Sogang University)

Production of medium-chain length polyhydroxyalkanoate from waste biomass

Hyung-Sool Lee

Korea Institute of Energy Technology, Canada

Polyhydroxyalkanoates (PHA) are a class of biodegradable polyesters that can be produced from microorganisms. It has significant potential for commercial application, and it is biodegradable in nature. In this study, we have reported PHA production by using Pseudomonas putida strain KT2440 (pmid:6282695) in a 5 L lab-scale bioreactor. We used an artificial fermentation broth (AFB) prepared with volatile fatty acid to mimic food waste fermentation. The initial VFA concentration in AFB consisted of butyrate 10.12±0.72 g/L; propionate 10.22±0.14 g/L; acetate 7.87±0.56 g/L; valerate 0.8 g/L; hexanoate 4.66 g/L. We have estimated PHA yield, and monomer composition, along with its physical, chemical, thermal, and mechanical properties. A biomass productivity of 8.69±0.45 was achieved with a VFA removal efficiency of 81.75±3.08%. The highest PHA productivity of (34.81±1.67%) was achieved in this study. Gas chromatography revealed that PHB contributes 83.6% to 86.1% of total PHA followed by PHH (6.6%-8.6%) and PH2MV (4.9%-8.3%). Thermogravimetric analysis (TGA) showed that PHA polymer started degrading at a temperature of 150°C and maximum polymer loss weight at a temperature of about 270°C. Differential scanning calorimeter (DSC) revealed two peaks corresponding to the melting temperature of the polymer i.e., temperature 1 (Tm1) at 140.6°C, and temperature 2 (Tm2) at 154.87° C. This indicates that the produced PHA polymer is a heteropolymer, a blend of copolymers, having two melting temperatures. This result will help to develop integrated PHA production processes within a circular biorefining concept, and it is the most likely way to achieve maximum economic and environmental benefit.

Symposium : **POLY3-4**

Recent Advances in Sustainable Polymer Materials

Room 302+303 FRI 15:55

Chair: Jeyoung Park (Sogang University)

Evaluation of biomass content and biocarbon in bioplastics and research using AMS

Hyeonyeol Jeon*, **Jeyoung Park**[1]

Korea Research Institute of Chemical Technology, Korea

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

Bioplastics have seen a rapid increase in interest and demand as one of the many ways to achieve carbon neutrality. As a sustainable material to replace petroleum-based plastics and to reduce CO_2 emissions, bioplastics based on biomass are a suitable material. In particular, bioplastic material manufacturing, biodegradability assessment for verification, and biomass content assessment are essential fields related to certification. Among them, biomass content evaluation is one of the analyses used to confirm this, as there is no difference between petroleum-based and biomass-based polymers in terms of chemical structure and properties, even if they are the same polymer. By using an accelerator mass spectrometer to analyze bio-carbon and ^{14}C, a naturally occurring radioactive carbon, present in biomass, it is possible to quantitatively analyze the presence of bioplastics and the content of biomass. It is widely used as a means to certify bioplastics in the United States and Europe based on ASTM 6866B, and in this study, we will introduce the analysis and research trends utilizing this accelerator mass spectrometry method.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **INOR1-1**
Recent Trends in Inorganic Materials Chemistry
Room 211+212+213 THU 15:40
Chair: Joohyun Lim (Kangwon National University)

Circularly polarized luminescence in coordination-driven assemblies

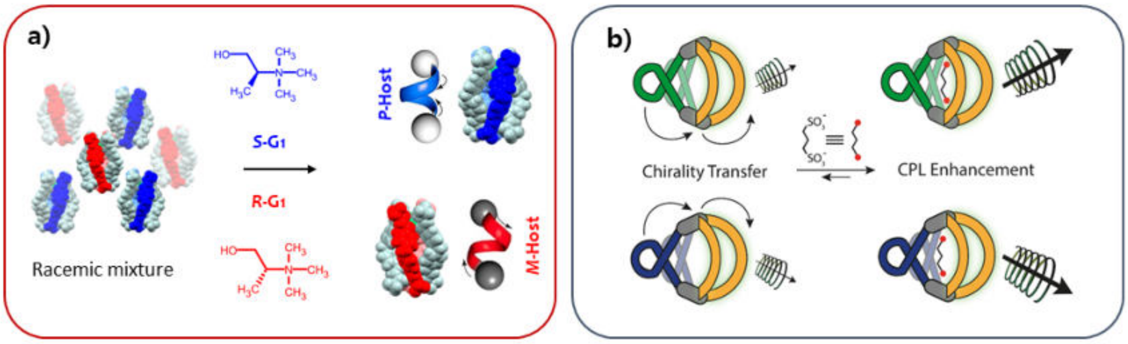
Jacopo Tessarolo

Department of Chemistry, Chonnam National University, Korea

Metal-mediated self-assembly of supramolecular architectures has been proven to be an efficient tool for developing new materials with well-defined shapes and geometries. Proper ligand design and choice of metal centers, allow to obtain a large variety of compounds with nanosized pockets able to host specific guest molecules [1]. At the same time, functions deriving from the metal center, such as lanthanide emission [2], or from the organic ligand, for instance chromophores or photoswitches [3], can be implemented to assemble multifunctional systems. Herein we combine chirality and emission properties from different building blocks, to achieve circular polarized luminescence (CPL) in supramolecular assemblies via guest-to-host [2] (Figure 1a) or ligand-to-ligand chirality transfer [4] (Figure 1b). The latter is based on the combination of multiple ligands following non-statistical processes to yield heteroleptic assemblies [5] displaying CPL. The presence of a cavity allows to study molecular recognition, while combining multiple ligands allows or to tune the properties of the systems by exchanging the building blocks in a modular fashion.

References:

[1] Clever G. H. et al. Chem. Soc. Rev., 2014, 43, 1848
[2] Rancan M.; Tessarolo J.; et al. Cell Reports Physical Science, 2022, 3, 100692
[3]Lee H.; Tessarolo J.; Clever G. H. et al. J. Am Chem. Soc., 2022, 144, 3099
[4] a) Wu K.; Tessarolo J.; Baksi A.; Clever, G. H., Angew. Chem. Int. Ed., 2022, 61, e202205725; b) Tessarolo J.; Clever G. H. et al. Chem. Comm., 2023, 59, 3467.
[5] Pullen S.; Tessarolo J.; Clever G. H., Chem. Sci., 2021, 12, 7269


a)
Racemic mixture
HO
CH3
N
CH3
H3C
CH3
S-G1
R-G1
P-Host
M-Host
b)
Chirality Transfer
CPL Enhancement
SO3-
SO3-
≡

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **INOR1-2**
Recent Trends in Inorganic Materials Chemistry
Room 211+212+213 THU 16:00
Chair: Joohyun Lim (Kangwon National University)

Porphyrin Box-based Supramolecular Architectures

Younghoon Kim

Center for Bio-based Chemistry, Korea Research Institute of Chemical Technology, Korea

In 2015, porphyrin boxes (PBs) using imine condensation reaction of six porphyrin units and eight trigonal building blocks were reported, and by virtue of their unique properties, PBs have been applied to interesting applications. First, the truncated cubic-shaped geometry and six porphyrin faces of PBs prompted us to explore metallated PBs as organic SBUs to build hierarchical superstructures by connecting them using ditopic bridging ligands. Using this approach, we obtained PB-based superstructures (PSS) with two-fold interpenetrated network and large surface area, which can be utilized as a heterogeneous catalyst for photooxidation of juglone. Second, we also reported a new supramolecular architecture consisting of a tightly packed square-planar core of four fullerenes surrounded by six Zn-PBs. This unique packing showed strong charge-transfer interactions between the two components, and formation of charge-separated states, which leads to extraordinarily long lifetimes in the excited state.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **INOR1-3**

Recent Trends in Inorganic Materials Chemistry

Room 211+212+213 THU 16:20

Chair: Joohyun Lim (Kangwon National University)

Ternary Cu–In–Se Quantum Dots for Improving Photoelectrochemical Hydrogen Generation by Defect Engineering

Su il In

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

Heavy-metal-free ternary CISe QDs are promising for solar fuel production because of their low toxicity, tunable band gap, and high light absorption coefficient. Although defects significantly affect the photophysical properties of QDs, the influence on photoelectrochemical hydrogen production is not well understood. Herein, we present the defect engineering of CISe QDs for efficient solar-energy conversion. Lewis acid–base reactions between metal halide–oleylamine complexes and oleylammonium selenocarbamate are modulated to achieve CISe QDs with the controlled amount of Cu vacancies without changing their morphology. Among them, CISe QDs with In/Cu = 1.55 show the most outstanding photoelectrochemical hydrogen generation with excellent photocurrent density of up to 10.7 mA cm^{-2}, attributed to the suitable electronic band structures and enhanced carrier concentrations/lifetimes of the QDs. The proposed method, which can effectively control the defects in heavy-metal-free ternary QDs, offers a deeper understanding of the effects of the defects and provides a practical approach to enhance photoelectrochemical hydrogen generation.

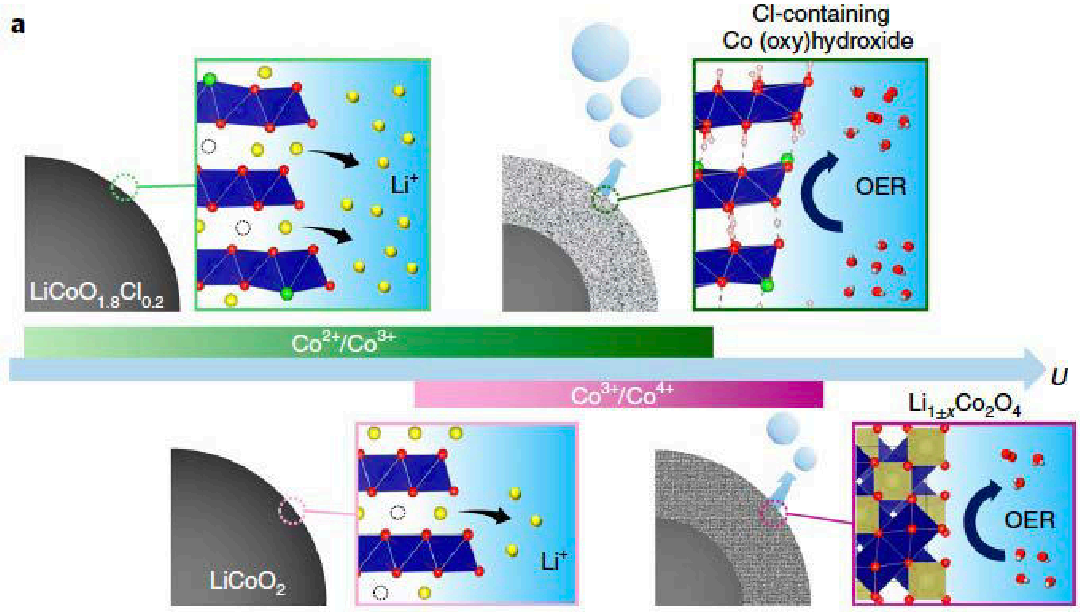
Symposium : **INOR1-4**
Recent Trends in Inorganic Materials Chemistry
Room 211+212+213 THU 16:45
Chair: Joohyun Lim (Kangwon National University)

Dynamic active surface phase evolution during electrochemical catalysis.

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

Revealing and redirecting the dynamic evolution of active species for efficient electrochemical catalytic reactions, such as water electrolysis and electrochemical CO_2 reduction (ECR), present significant challenges. In my talk, I will introduce a cationic redox-tuning method to modulate in situ catalyst leaching and to redirect the dynamic surface restructuring of $LiCoO_{2-x}Cl_x$ ($x = 0$, 0.1, or 0.2) for the electrochemical oxygen evolution reaction (OER). We found that chlorine doping lowers the potential needed to trigger in situ cobalt oxidation and lithium leaching. This leads to the transformation of the surface of $LiCoO_{1.8}Cl_{0.2}$ into a self-terminated amorphous (oxy)hydroxide phase during OER. In the second part of my talk, I will focus on electrochemical CO_2 reduction. Here, we directly observed the chemical and morphological evolution of highly efficient ECR catalysts during operation. We identified key intermediate species that contribute to highly active surfaces and significantly enhance C–C coupling activity. Utilizing operando transmission soft X-ray microscopy, we visualized the nanoscale chemical composition distribution of Cu-based catalysts during ECR. Our observations revealed that partially evolved Cu^+ phases and surface Cu^{2+} phases are responsible for the dynamic dissolution–redeposition process and high C–C coupling activity, respectively. We further demonstrated that this dissolution–redeposition process is electrochemically triggered by inducing Cu^+ phases, which are redirected to malachite (Cu^{2+}) phases even under high cathodic potentials.


a
Cl-containing
Co (oxy)hydroxide
Li+
OER
LiCoO1.8Cl0.2
Co2+/Co3+
U
Co3+/Co4+
Li1±xCo2O4
Li+
OER
LiCoO2

Symposium : **INOR1-5**

Recent Trends in Inorganic Materials Chemistry

Room 211+212+213 THU 17:10

Chair: Joohyun Lim (Kangwon National University)

Generation and Storing of H_2 Using Inorganic Nanomaterials

Minyoung Yoon

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

Due to global climate change, using non-carbon sources as an energy source is required, and H_2 can be a candidate to replace fossil fuels. Considering the full cycle of H_2 technology, production and delivery/storage are critical issues to tackle. Considering production, current production is mainly dependent on fossil fuel-dependent technology. However, the development of electrocatalytic and photocatalytic H_2 production technology should be developed. In addition, a new technology should be developed for the facile delivery and storage of H_2. Inorganic materials can provide unique solutions for H_2 generation and delivery/storage. Herein, we present a diatom/NiS composite material for the generation of H_2. The HER activity was significantly enhanced when the NiS was composited with naturally occurring microalgae (diatoms). Due to the effect of the porous 3D structure of diatom, the NiS can show a synergetic effect in hydrogen evolution reaction (HER). The enhanced HER performance was studied by DFT calculation to understand the mechanism. Unlike the generation of H_2, the storage process requires the development of storage media (liquid organic hydrogen carrier; LOHC) and hydrogenation/dehydrogenation catalysts. A novel organic media, methylbenzyl naphthalene (MBN), was newly prepared on a large scale (> 10 g). For the storage and extraction of H_2, new Pt and Ru nanocatalysts were developed for hydrogenation and dehydrogenation, respectively, was developed. The MBN showed the lowest dehydrogenation enthalpy among homocyclic LOHC media, which allows facile dehydrogenation of the media.

Symposium : **INOR2-1**
Recent Advances in Organometallic Chemistry and Coordination Chemistry
Room 211+212+213 FRI 09:00
Chair: Jin Yeong Kim (Seoul National University)

Chemical Space Expedition to Target Materials Discovery for Carbon Neutrality

Wonyoung Choe

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

The demand for high-performance materials for global sustainability is high. Despite such urgent demand, the development of new materials is rather slow, compared to recent technological advancements in other areas such as computer industries. To overcome such a bottleneck situation, we need revolutionary approaches in the design, synthesis, and characterization of new materials. In this presentation, as an attempt to accelerate materials discovery, I will present a blueprint for zeolite imidazolate frameworks, an important class of materials in gas separation, together with synthetic strategies. A similar approach can be extended to Zr-based metal-organic frameworks. We expect that such an endeavor will result in CO2 reduction by 2050.

Symposium : **INOR2-2**
Recent Advances in Organometallic Chemistry and Coordination Chemistry
Room 211+212+213 FRI 09:25
Chair: Jin Yeong Kim (Seoul National University)

Achieving Efficient TADF Using Rigid Boron Compounds

Min Hyung Lee

Department of Chemistry, University of Ulsan, Korea

Thermally activated delayed fluorescence (TADF) compounds have attracted considerable attention as efficient emitters in organic light-emitting diodes (OLEDs) because they can achieve nearly 100% internal quantum efficiency through efficient triplet-to-singlet upconversion via reverse intersystem crossing (RISC). Thanks to the highly emissive properties and strong electron-accepting nature of the triarylboryl moieties, boron-based compounds have emerged as the most promising emitters in OLEDs. Several factors should be considered for the design of efficient boron-based TADF emitters; i) enhancing the rate of the RISC process, ii) high photoluminescent quantum yields (PLQYs), and iii) rigid and stable molecular structures. To this end, we have developed rigid boron-based TADF emitters with spiro-donor-acceptor and sterically shielded multi-resonance structures. Using these compounds as emitters, we have realized high efficiency blue OLEDs with reduced efficiency roll-offs. The details of the design, synthesis, and photophysical and electroluminescent properties of the emitters will be presented.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **INOR2-3**
Recent Advances in Organometallic Chemistry and Coordination Chemistry
Room 211+212+213 FRI 09:50
Chair: Jin Yeong Kim (Seoul National University)

Conductive Metal-Organic Framework Thin Films

Sarah Sunah Park

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

Developing conducting metal−organic frameworks (MOFs) provides an avenue for creating high surface area conductors with potential applications ranging from electrocatalysts and chemiresistive sensors to supercapacitors. Highly ordered and infinite charge transport pathways could be realized in conducting MOF platforms to yield high conductivity. However, it is challenging to engineer electrical conductivity in MOFs because these materials generally have flat bands determined by highly localized organic states and weak hybridization with the inorganic units. Based on using intermolecular π-stacking interactions as topology defining factors of MOFs, strategies for synthesizing and utilizing the conductive and microporous MOFs will be discussed. In addition, the synthesis of a conductive two-dimensional MOF thin film by single-step all-vapor-phase chemical vapor deposition will be presented. The large-area thin film of $Cu_3(C_6O_6)_2$ synthesized in this study has high crystallinity and an edge-on-orientation. Using e-beam lithography, microdevices based on $Cu_3(C_6O_6)_2$ thin film were fabricated, which showed an electrical conductivity of 92.95 S/cm. The synthesis of conductive MOF thin films through all-vapor-phase CVD could provide insights into the physical properties of these materials and pave the way for their practical applications.

Symposium : **INOR2-4**

Recent Advances in Organometallic Chemistry and Coordination Chemistry

Room 211+212+213 FRI 10:15

Chair: Jin Yeong Kim (Seoul National University)

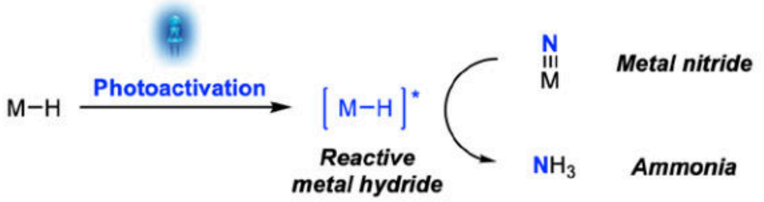
Two Approaches to Generate and Utilize Reactive Inorganic Intermediates: Photo- and Redox-Activation

Sangmin Kim

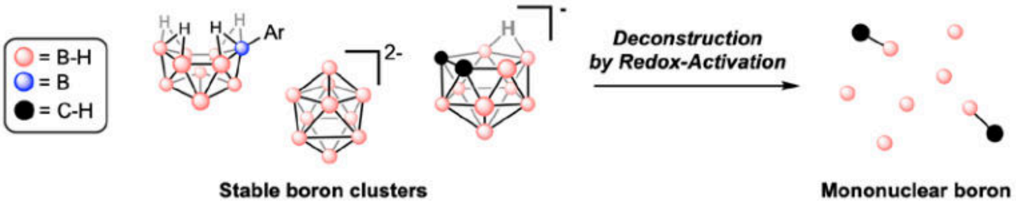
Department of Chemistry, Yonsei University, Korea

Reaction intermediates are a crucial element in various chemical reactions, including a wide range of synthetic and catalytic reactions. Consequently, generating highly reactive intermediates can provide access to new reactions that are thermodynamically challenging to approach by conventional methods. In this presentation, I will demonstrate two main strategies to generate reactive inorganic intermediates: photo and redox activation, and how to utilize them to develop unprecedented and challenging reactions.Some Cp*-based transition metal hydrides can serve as hydrogen atom transfer (HAT) mediators, where the new bond to be formed should be stronger than a M(metal)-H bond due to thermodynamic reasons. However, because most metal hydrides have a M-H bond dissociation free energy (BDFE) higher than 52 kcal/mol, it has been challenging to form an X-H bond weaker than 52 kcal/mol via HAT by transition metal hydrides. We have developed a strategy to harness photoactivation of transition metal hydrides to decrease the M-H BDFE to 21 kcal/mol and utilized it for formation of weak N-H bonds in the N2 reduction cycle to make NH3 using H2 as the hydrogen atom source.Moving on, boron clusters are much more readily accessible compounds from borohydride precursors compared to other commonly used boron reagents such as diboron species. Despite their accessibility, as well as their unique reactivity, their use as boron reagents has been limited due to their confined utilization. We have found that redox activation of boron clusters forms unstable intermediates, leading to the deconstruction of the boron cages to make synthetically useful mononuclear boron-based species such as boronic esters.

■ Photo-activation of Metal Hydrides to Promote Hydrogen Atom Transfer (HAT)



■ Redox-activation of Boron Clusters to Induce Boron-Cage Deconstructions



Symposium : **INOR2-5**

Recent Advances in Organometallic Chemistry and Coordination Chemistry

Room 211+212+213 FRI 10:35

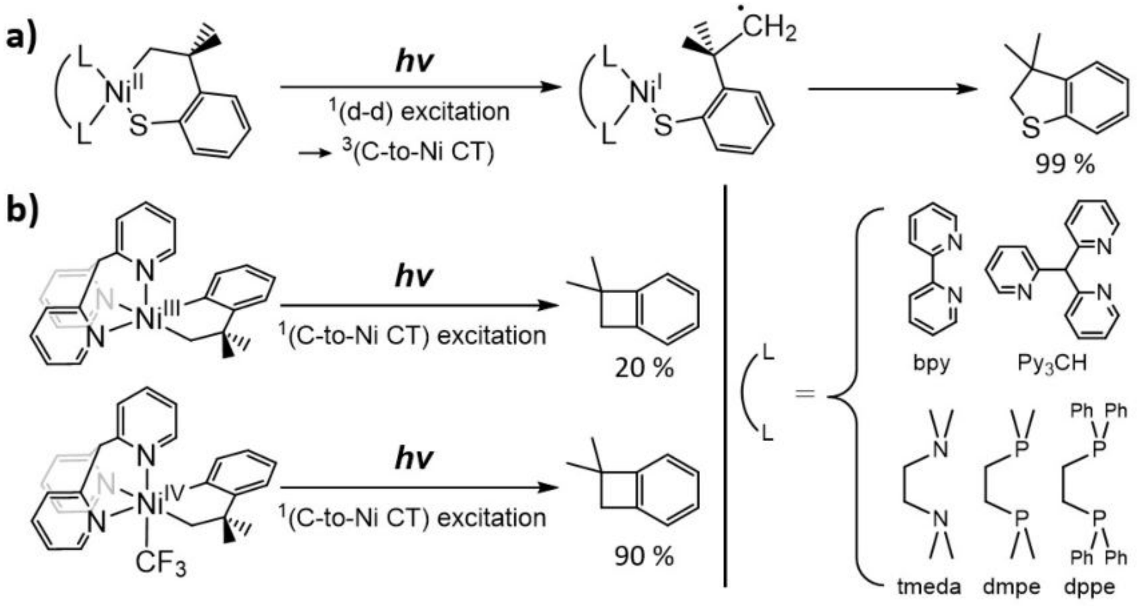
Chair: Jin Yeong Kim (Seoul National University)

Promotion of reductive elimination reactions by generating C-to-Ni charge-transfer excited states of organometallic $Ni^{II/III/IV}$ complexes

Jeongcheol Shin

Department of Chemistry, Duksung Women's University, Korea

While photoexcitation had become one of the acknowledged methods to activate Ni-catalyzed cross-coupling reactions, factors that determine the photoactivity of organonickel complexes are still under investigation. In this presentation, the C-to-Ni charge transfer (CT) states were proposed as key excited states for photo-induced reductive elimination (RE) reactions of nickelacycles, merging two different examples of photo-induced RE reactions: 1) *C-S bond-forming RE reactions of* Ni^{II} *complexes* and 2) *C-C bond-forming RE reactions of* Ni^{III} *and* Ni^{IV} *complexes*. The excited-state RE activities of nickelacycles with the thiacycloneophyl ligand have been measured with five different ancillary ligands, revealing that the RE activities depend on the excitation energy and are independent of the ancillary ligand. The electronic structural analyses utilizing electronic absorption (Abs) and magnetic circular dichroism (MCD) spectroscopies in combination with DFT computations have uncovered that d-d excitations can facilitate Ni-C bond homolysis to generate Ni^{I} intermediate via intersystem crossing to a dissociative ^{3}(C-to-Ni CT) state. The sequential C-S bond formation eventually produces the cross-coupled product. Alternatively, with cycloneophyl Ni^{III} and Ni^{IV} complexes, C-to-Ni CT excited states are directly accessible by visible light excitation, exhibiting 10^{5}-time enhanced RE activity compared to the ground state. These studies emphasize that the RE reactions can be promoted by accessing C-to-Ni CT excited states, and thus assist the design of Ni-catalyzed cross-coupling reactions incorporating photoexcitations.


a)
L
Ni^II
S
L
hν
1(d-d) excitation
→ 3(C-to-Ni CT)
CH2
Ni^I
S
99 %
b)
N
Ni^III
hν
1(C-to-Ni CT) excitation
20 %
Ni^IV
CF3
hν
1(C-to-Ni CT) excitation
90 %
L
L
=
N
bpy
Py3CH
N
tmeda
P
dmpe
Ph Ph
Ph Ph
dppe

Symposium : **INOR3-1**
Recent Trends in Nanochemistry Research
Room 211+212+213 FRI 14:30
Chair: Jeong-Eun Park (GIST)

Nanocrystal Chemistry within Atomic-Thin 2D-Slit-Nanospace

In Su Lee

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

Over the past years, our research has been pursuing the "nanospace-confined chemical reaction (NCCR) approach” which have explored the use of variety of solid and hollow silica-nanoparticles as either solid-state or solution-phase reaction medium to carry out the spatially confined syntheses and transformations of nanocrystals (NCs). This NCCR strategy offered the opportunity to observe and elucidate novel deconvoluted chemical phenomena that are impossible to investigate in bulk systems and also provided novel synthetic methodologies enabling us to access unprecedented functional nanomaterials. Recently, we could expand the scope of NCCR strategy, initially conducted with spherical nanospace, to 2-D anisotropic nanospace that could be templated by layered double hydroxides with nanometer-thickness. And, this study provided an in-depth understanding of the evolution and conversion chemistry of included NCs, which is highly influenced by the few-nm thickness of the 2D-nanospaces. In this talk, I will describe our recent efforts to develop 2D-platforms for NCCR study, highlighting new findings on completely reversible NC-conversion chemistry and highly oriented crystal growth with exposing unusual crystal surface, which are ascribed to the nanospace-confinement effect within the atomic-thin 2D-slit-nanospace.

Symposium : **INOR3-2**

Recent Trends in Nanochemistry Research

Room 211+212+213 FRI 14:55

Chair: Jeong-Eun Park (GIST)

Organelle-Targeted Fluorescent Nanodiamond Quantum Thermometry for Investigating Intracellular Metabolism

Jin Seok Lee

Department of Chemistry, Hanyang University, Korea

Intracellular thermometry serves as an influential tool for investigating biological processes and comprehending the thermogenesis dynamics in cells under specific physiological conditions. In particular, the role and biological process of organs in cells for various life activities are different and carried out independently, so the technology to measure temperature changes within certain organs is very important and expected to have a great impact. However, the development of biocompatible thermometers capable of independently assessing temperature changes in particular organelles during biological processes in living cells remains a significant challenge. In this study, we present the utilization of organelle-targeted nanodiamond quantum thermometry, employing nitrogen-vacancy color centers, for the monitoring of temperature changes in living fibroblasts cells during generation of ATP, a biological energy source. To accomplish this, we developed a microscopic system for studying intracellular heat generation in living cells using nanodiamond incorporating an incubating chamber system integrated with coplanar waveguides (CPWs) and a real-time nanodiamond tracking system. In particular, after fluorescent nanodiamonds were targeted in each of the three organelles, changes in temperature during ATP synthesis inhibition were monitored for each organelle. Our organelle-specific quantum thermometry technique has the potential to yield new insights into intracellular metabolism and the temperature variations occurring in specific organelles and could be a valuable tool for studying biological processes in living cells.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **INOR3-3**
Recent Trends in Nanochemistry Research
Room 211+212+213 FRI 15:20
Chair: Jeong-Eun Park (GIST)

Plasmonic photothermal-based molecular diagnostics

Jung-hoon Lee

Department of Chemistry, Soonchunhyang University, Korea

For many biomedical research, polymerase chain reaction has been one of the most effective technologies. However, the thermocycling method used in modern PCR technology requires time-consuming and expensive Peltier-block heating. Many methods, including mechanical manipulation, microfluidics, and nano-sized droplets, have been examined and studied in an effort to address and replace these problems. Regarding the creation of devices and intricate sample preparation, there are still a number of significant restrictions. The photothermal effect is a phenomena wherein nanoparticles transform the energy of absorbed photons into thermal energy. The plasmonic photothermal-based nanoparticles are anticipated to exhibit tremendous potential for the development of nucleic acid amplification-based biosensors due to their strong and controllable optical characteristics, high spatiotemporal resolution, and high spatial and temporal resolution. I introduce a unique plasmonic photothermal-based PCR test for fast, low-cost, and precise detection in this talk.

Symposium : **INOR3-4**

Recent Trends in Nanochemistry Research

Room 211+212+213 FRI 15:40

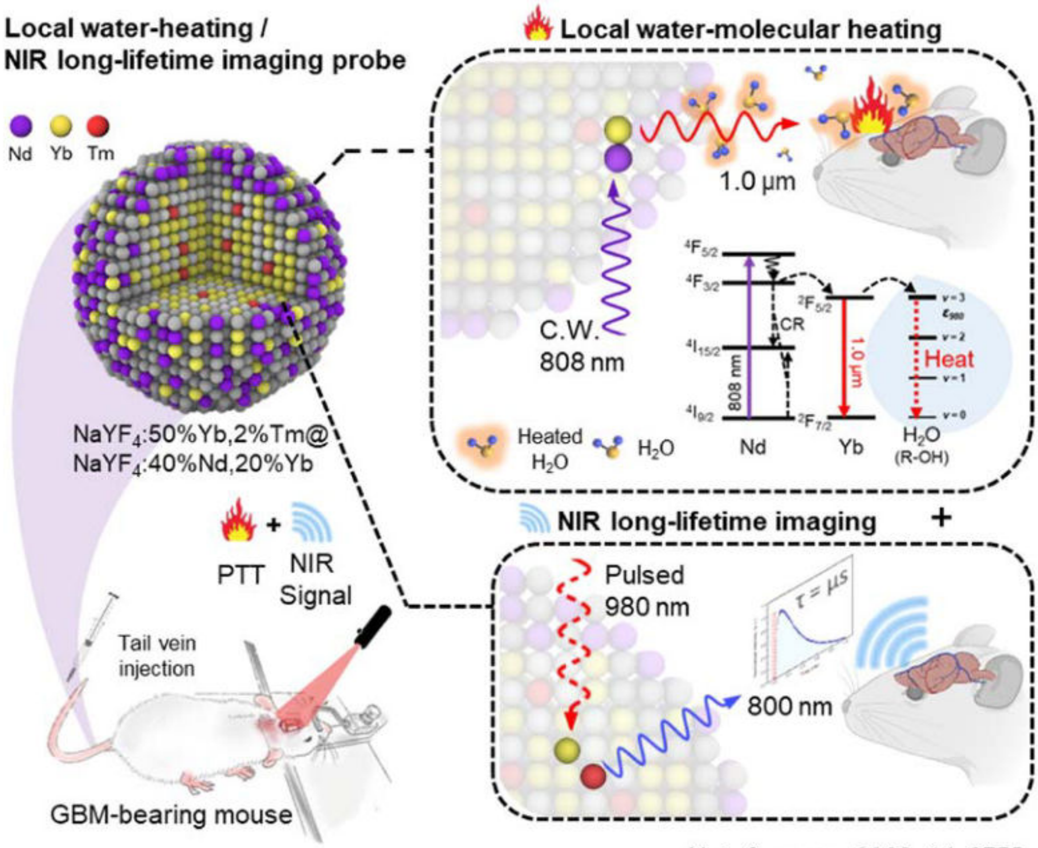
Chair: Jeong-Eun Park (GIST)

A Local Water Molecular-heating Strategy for Near-infrared Long-lifetime Imaging-guided Photothermal Therapy

Joonseok Lee

Chemistry, Hanyang University, Korea

Owing to the strong absorption of water in the near-infrared (NIR) region near 1.0 μm, this wavelength is considered unsuitable as an imaging and analytical signal in biological environments. However, 1.0 μm NIR can be converted into heat and used as a local water-molecular heating strategy for the photothermal therapy of biological tissues. Herein, we describe a Nd-Yb co-doped nanomaterial (water-heating nanoparticles (NPs)) as strong 1.0 μm emissive NPs to target the absorption band of water. Furthermore, introducing Tm ions into the water-heating NPs improve the NIR lifetime, enabling the development of a NIR imaging-guided water-heating probe (water-heating NIR NPs). In the glioblastoma multiforme male mouse model, tumor-targeted water-heating NIR NPs reduce the tumor volume by 78.9% in the presence of high-resolution intracranial NIR long-lifetime imaging. Hence, water-heating NIR NPs can be used as a promising nanomaterial for imaging and photothermal ablation in deep-tissue-bearing tumor therapy.



Nat. Commun. **2023**, 14, 2755

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **INOR3-5**
Recent Trends in Nanochemistry Research
Room 211+212+213 FRI 16:05
Chair: Jeong-Eun Park (GIST)

Epitaxial Growth of 2D MoS2 and WS2 using inorganic molecular precursors, MOCl4 and WOCl4: The critical role of Substrate Surface Termination

Hyunseob Lim

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

This study demonstrate the exceptional chemical route for synthesizing uniform and large-area films of monolayer MoS2 and WS2, ones of representative transition metal dichalcogenides. The conventional precursors for MoS2 and WS2 synthesis by chemical vapor deposition (CVD), such as solid-state metal oxides or metal-organic molecules causes the several drawbacks, like the deficient reproducibility and the inevitable carbon contaminations. To overcome these limitations, we developed the inorganic molecular CVD method using inorganic molecular precursors, MOCl4 and WOCl4, with gaseous sulfur precursor, H2S, which enables the precise control of the partial pressure for all precursors during CVD process. Consequently, the of high-quality and carbon-free MoS2 and WS2 films can be synthesized only for several tens of minutes. In addition, the epitaxial growth of MoS2 film was successfully demonstrated, which exhibited excellent electrical and optical properties, outstanding homogeneity, and orientation selectivity. The systematic investigation of the effect of growth temperature on the crystallographic orientations of MoS2 revealed that the surface termination of the sapphire substrate depending on the growth temperature, plays a critical role in determining the crystallographic orientation selectivity of MoS2. The elaborate surface characterizations combined with theoretical calculations suggested that the formation of half-Al-terminated surface at a high temperature is crucial for the epitaxial growth of MoS2 on a C-plane sapphire substrate. We believe that the extended knowledges by our work, regarding the roles of the substrate surface termination on the epitaxial growth, will highly contribute to designing the efficient epitaxial growth routes for single crystalline 2D materials.


사단법인 대한화학회
KOREAN CHEMICAL SOCIETY

Award Lecture in Division : **PHYS1-1**

Recent Physical Chemistry Studies on Photo/Electrochemistry

Room 208+209+210 THU 15:40

Chair: Kyungwon Kwak (Korea University)

Plasmonic Nanoparticle Assembly: A Journey to Explore Optical, Electronic, and Thermal Properties Arising from Au Nanogaps

Sangwoon Yoon

Department of Chemistry, Chung-Ang University, Korea

Plasmon refers to a collective oscillation of conduction electrons in gold nanoparticles (AuNPs) coupled to external electromagnetic fields. Plasmon accounts for most of the unique properties of AuNPs such as their vivid red colors in dispersion, generation of local electric fields around the nanoparticles, production of hot charge carriers, and photoinduced heating. Each property offers immense application potentials in display, colorimetric sensing, surface-enhanced spectroscopy, photocatalysis, photovoltaics, and photothermal therapy, to name a few. Interestingly, these properties are significantly enhanced in narrow nanogaps between the AuNPs. Thus, creation of nanogaps is the key to fully exploring the plasmonic properties of AuNPs. We note that nanogaps are naturally formed when the individual nanoparticles are put together to form an assembly structure. In this spirit, my group has focused on producing many combinations of AuNP assemblies with various shapes and sizes. The high-yield, well-controlled AuNP assemblies allow us to examine closely the relationship between the nanogap parameters and the plasmonic properties represented by plasmon coupling, Raman enhancement, and hot carrier generation efficiency. In this honorary presentation, I would like to share my group’s collective efforts in this journey and the highs and lows that we encountered along the way.

Symposium : **PHYS1-2**

Recent Physical Chemistry Studies on Photo/Electrochemistry

Room 208+209+210 THU 16:10

Chair: Yun Jeong Hwang (Seoul National University)

Direct observation of ammonia & water oxidation on photoanode

Wooyul Kim

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

Metal oxide based semiconductor is widely recognized as a highly promising material for water photo-oxidation, primarily due to its ability to absorb visible light. However, it faces inherent limitations in generating peroxo species, maintaining stability, and preventing the recombination of surface defect sites. Various strategies are currently being employed to overcome these limitations, including surface passivation, control of oxygen vacancies, and the chemical and physical deposition of co-catalysts. Here, we investigated the effects of passivating overlayers on WO3 and BiVO4 electrodes. We utilized WO3 electrodes prepared through electrodeposition, as well as composite electrodes Al2O3/WO3 and TiO2/WO3 prepared via atomic layer deposition (ALD). Our investigation involved both photoelectrochemical activity assessment and laser flash photolysis measurements to study the dynamics of charge carriers. Our findings demonstrate distinct photoelectrochemical outcomes based on the passivating materials used. Notably, femtosecond to microsecond transient absorption spectroscopy of WO3, Al2O3/WO3, and TiO2/WO3 revealed an ultra-fast pathway for charge carriers in the presence of Al2O3 and TiO2 overlayers (on the order of picoseconds) under applied bias conditions. Conversely, the relatively long-lived trapped hole fraction increased with the presence of the overlayers (on the order of seconds), thereby promoting water photooxidation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **PHYS1-3**

Recent Physical Chemistry Studies on Photo/Electrochemistry

Room 208+209+210 THU 16:30

Chair: Yun Jeong Hwang (Seoul National University)

Electrochemical CO_2 Reduction using Palladium-based electrocatalysts

Ji Hoon Lee

School of Materials Science and Engineering, Kyungpook National University, Korea

Electrochemical CO_2 reduction reactions (CO_2RR) have gained much attention in the past decades. Especially, when coupled with renewable energy resources, it can play an important role in realizing a sustainable energy cycle toward the net reduction of carbon emissions by producing valuable chemicals while reducing CO_2.In this talk, I will introduce my recent works on palladium (Pd)-based CO_2 electrocatalysts with a focus on their structure-dependent reaction pathway. It is well-known that Pd is readily poisoned by carbon monoxide (CO), thus producing formic acid (HCOOH) at low electrochemical potentials for CO_2RR. However, it was found that, once it transformed into Pd hydride (PdH), it was able to produce CO with tunable syngas (CO/H_2) ratios. Such structure (Pd/PdH)-product (HCOOH/CO) relationship was further corroborated by using in-situ X-ray diffraction (XRD) and X-ray fine absorption structure (XAFS) analyses. Together with density functional theory (DFT) calculations, the Gibbs energy difference of *H and *HOCO, which are the first reaction intermediates for CO and H_2 evolution reactions, respectively, is identified as the key descriptor for syngas production with tunable ratios. Secondly, I will introduce Pd-based single-atom catalysts (SACs) as a new cost-effective Pd-based electrocatalyst. By correlating in-situ X-ray characterizations and DFT calculations, a comprehensive understanding of the physicochemical properties of Pd-based nanoparticles and SACs will be presented. Finally, ongoing efforts to probe surface reactions using in-situ characterizations in my group will be introduced.

Symposium : **PHYS1-4**

Recent Physical Chemistry Studies on Photo/Electrochemistry

Room 208+209+210 THU 16:50

Chair: Yun Jeong Hwang (Seoul National University)

Importance of charge transfer descriptor for the computational screening of electrocatalysts

Stefan Ringe

Chemistry, Korea University, Korea

Electrochemistry has become a key player in establishing a global sustainable energy landscape. Unfortunately, most electrochemical processes are limited in their efficiency and selectivity which has prevented them from replacing carbon-intensive industrial processes. Computational simulations can help on various sides to improve electrochemistry, from the fundamental, atomistic understanding, over multi-scale modeling of realistic devices up to high-throughput screening of electrocatalysts. In this talk, I want to focus in particular on electrochemical CO2 reduction and the importance of accounting for the electrochemical environment when screening electrocatalysts. We find that descriptors depicting the charge-transfer characteristics of potential catalysts is essential for developing optimized materials.

Symposium : **PHYS1-5**

Recent Physical Chemistry Studies on Photo/Electrochemistry

Room 208+209+210 THU 17:10

Chair: Yun Jeong Hwang (Seoul National University)

Understanding of the Polarization-Induced Interfacial Microenvironments

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.

Symposium : **PHYS2-1**
Computers and Chemistry: Recent Research Trends
Room 208+209+210 FRI 09:00
Chair: Hyungjun Kim (KAIST)

Exploring Physical and Chemical Space of Molecular Systems from First Principles: Human and/or Artificial Intelligence

Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Molecular systems have a diverse range of physical and chemical properties which are often correlated with their structures. Over the last 15 years, we have been developing a series of theoretical and computational schemes to assist our understanding on the structure-property correlations using both human and artificial intelligence. For example, the complex hydrogen-bond pattern in water/methanol has been extensively investigated by experimental means1-2, however interpretation of these data is not possible without the assistance of artificial intelligence algorithms (such as genetic algorithms), multi-scale methods and recently to neural network potential3-6. Recently, our group has initiated a joint project on the application of mass spectrometry for quick identifications different types of saccharides, the underlying dissociation mechanisms can be analyzed by engaging huge number of ab initio calculations. However, to understand both of the physics and chemistry of sugar requires addition assistance from both human and artificial intelligence6-10.

References:
1.J. Chem. Phys. 122, 74315 (2005)
2.Phys. Chem. Chem. Phys., 20, 14971-14991 (2018)
3.J.Chem. Phys. 122, 24516 (2005)
4.J. Chem. Theory and Comp. 5, 2629 (2009)
5.Phys. Chem. Chem. Phys. (Accepted)
6.Phys. Chem. Chem. Phys., 20, 19614-19624 (2018)

7.J. Phys. Chem, A 123, 3441 (2019)

8.Phys. Chem. Chem. Phys., 24, 27263 (2022)

9.Phys. Chem. Chem. Phys., 25, 5817 (2023)

10.Phys. Chem. Chem. Phys., 25, 3352 (2023)

Symposium : **PHYS2-2**

Computers and Chemistry: Recent Research Trends

Room 208+209+210 FRI 09:20

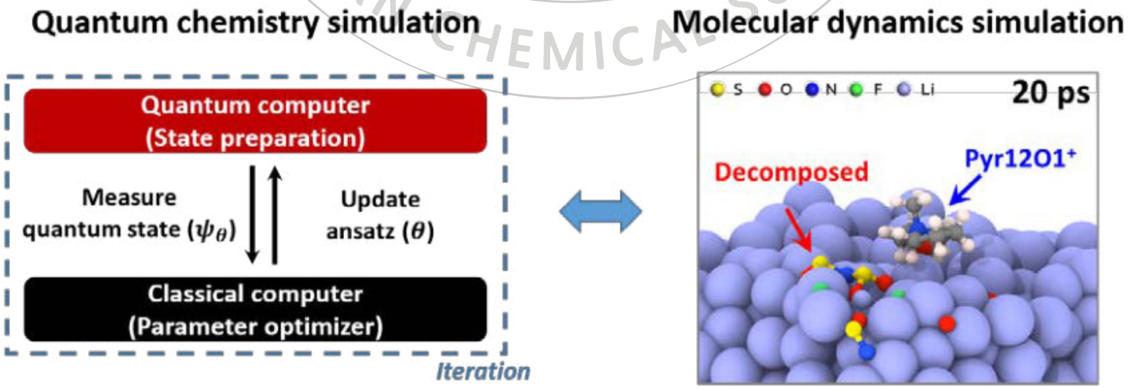
Chair: Hyungjun Kim (KAIST)

Quantum computing and molecular simulation studies on the industrial side

Kyujin Shin

Computational Materials Research Team, Hyundai Motor Company, Korea

The presentation is structured as follows. The talk begins by introducing the quantum algorithm for solving electronic structure problems on near-term quantum computers. In this work, we consider an orbital-optimized pair-correlated approximation to the unitary coupled cluster with singles and doubles (uCCSD) ansatz for the variational quantum eigensolver (VQE) and report a highly efficient quantum circuit implementation for trapped-ion quantum computers. It concludes with a summary of our current studies on the quantum and molecular simulations of electrocatalyst and electrolyte.



Symposium : **PHYS2-3**
Computers and Chemistry: Recent Research Trends
Room 208+209+210 FRI 09:40
Chair: Hyungjun Kim (KAIST)

DFT Study on Interface Electronic Structure

Geunsik Lee

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

Overall performance of various types of energy conversion and quantum devices is driven by interface properties as well as properties of active materials. Experimental characterizations of interface to correlate with or improve device performance is challenging and costs highly. Meanwhile, theoretical modeling can provide valuable information towards high performance devices. Among various theoretical approaches, the density functional theory (DFT) method is remained very useful to understand the observed physical and chemical properties based on details of electronic structure at the interface. Here, it will be presented how DFT calculations could be helpful to give valuable insight. Examples will include electrocatalytic reaction at the interface, magnetic/electronic structure of van der Waals materials. It will be also shown that surface or interface electronic structure is important to understand materials properties, thus it should be considered properly in addition to bulk properties to describe target properties of materials.

Symposium : **PHYS2-4**

Computers and Chemistry: Recent Research Trends

Room 208+209+210 FRI 10:00

Chair: Hyungjun Kim (KAIST)

Reducing metal-semiconductor contact resistance by inserting two-dimensional material

Yeonchoo Cho

Samsung Advanced Institute of Technology, Korea

In a field-effect transistor, reducing the metal-semiconductor contact resistance is a key to reducing power consumption and increase the operation speed. In order to achieve this goal, the energy barrier, the so-called Schottky barrier, needs to be thinned and lowered. Traditionally, achieving this has involved heavily doping the semiconductor to thin the Schottky barrier. In this talk, we show that the Schottky barrier height can be controlled by inserting a two-dimensional material at the metal-semiconductor interface. [1, 2] In addition, in the case of a two-dimensional semiconductor, we show that modulation doping can be employed to control the Schottky barrier height. [3][1] M.H. Lee, Y. Cho et al. Nano Lett. 18, 4878 (2018)[2] S.G. Nam, Y. Cho et al. 2D Mater. 5, 041004 (2018)[3] Y. Cho et al. Nano Lett. 22, 9700 (2022)

Symposium : **PHYS2-5**

Computers and Chemistry: Recent Research Trends

Room 208+209+210 FRI 10:20

Chair: Hyungjun Kim (KAIST)

Active Learning approach in designing entropy alloy nanocatalyst

YongJoo Kim

Department of Materials Science and Engineering, Kookmin University, Korea

Design of bifunctional multimetallic alloy catalysts, which are one of the most promising candidates for water splitting, is a significant issue for the efficient production of renewable energy. Owing to large dimensions of the components and composition of multimetallic alloys, as well as the trade-off behavior in terms of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) overpotentials for bifunctional catalysts, it is difficult to search for high-performance bifunctional catalysts with multimetallic alloys using conventional trial-and-error experiments. Here, an optimal bifunctional catalyst for water splitting is obtained by combining Pareto active learning and experiments, where 110 experimental data points out of 77946 possible points lead to effective model development. The as-obtained bifunctional catalysts for HER and OER exhibit high performance, which is revealed by model development using Pareto active learning; among the catalysts, an optimal catalyst (Pt0.15Pd0.30Ru0.30Cu0.25) exhibits a water splitting behavior of 1.56 V at a current density of 10 mA cm−2. This study opens avenues for the efficient exploration of multimetallic alloys, which can be applied in multifunctional catalysts as well as in other applications.

Symposium : **PHYS2-6**
Computers and Chemistry: Recent Research Trends
Room 208+209+210 FRI 10:40
Chair: Hyungjun Kim (KAIST)

Autonomous Laboratory for Bespoke Synthesis of Nanoparticles

Sang soo Han

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

The optimization of nanomaterial synthesis with numerous synthetic variables is often considered an extremely difficult task because the conventional combinatorial explorations are prohibitively expensive. In this work, we report the autonomous experimentation system platform developed for the bespoke design of nanoparticles (NPs) with target optical properties. This system platform operates in a closed-loop manner between NP batch synthesis module of NPs and UV-Vis spectroscopy module, based on the feedback of the AI optimization modeling. With silver (Ag) NPs as a representative example, we demonstrate that the Bayesian optimizer implemented with the early stopping criterion can efficiently produce Ag NPs precisely possessing the desired absorption spectrums within only 200 iterations when optimizing five synthetic reagents. Besides the outstanding material developmental efficiency, the analysis of synthetic variables further reveals a previously unknown chemistry regarding the effects of citrate in Ag NP synthesis. The amount of citrate is a key to controlling the competitions between spherical and plate-shaped NPs, and as a result affects the shapes of absorption spectrums as well. Our study highlights both enhancing search efficiencies and providing a novel knowledge of the revelation of citrate effects by analyzing the datasets accumulated from the autonomous experimentation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Recent Advances in Physical Chemistry for Energy Science

Room 208+209+210 FRI 14:20

Chair: Kyungwon Kwak (Korea University)

Anion and Cation in Neurodegenerative Diseases

Sang Hak Lee

Department of Chemistry, Pusan National University, Korea

The study of non-bonding interactions has transcended the exclusive domain of physical chemists employing spectroscopy and computer simulations. With the advent of molecular biology, non-bonding interactions have emerged as pivotal factors in comprehending the structures and functionalities of biomolecules, including DNA and proteins. Among these non-bonding interactions, ionic interactions stand out as the most robust forces mediating interactions between anionic and cationic molecules. When scrutinizing the intracellular milieu, non-bonding interactions, particularly those of the ionic nature, wield significant influence over protein-protein and DNA-protein interactions. Consequently, we hypothesized that protein aggregation or phase separation, known contributors to neurodegenerative diseases such as Alzheimer's, Parkinson's, and Lou Gehrig's diseases, may also be governed by these ionic interactions. Given the highly charged nature of disease-related proteins, a substantial charge disparity exists, making self-aggregation in the absence of cofactors a formidable challenge. Our research has yielded a compelling insight: small charged biomolecules play a pivotal role in facilitating the formation of protein condensates through ionic interactions within cellular environments.

Award Lecture in Division : **PHYS3-2**

Recent Advances in Physical Chemistry for Energy Science

Room 208+209+210 FRI 14:45

Chair: Kyungwon Kwak (Korea University)

Unconventional NMR Spectroscopy: Analysis of Proteins in Erythrocytes

Jung Ho Lee

Department of Chemistry, Seoul National University, Korea

NMR spectroscopy has been around for 80 years. I find the field exciting as method developments continue to push the boundaries of what can be achieved by NMR. One of its unique applications is In-cell NMR, which uses the non-destructive nature of NMR to investigate molecules in live cells. Here, we present the first instance of protein NMR in human-derived cells; erythrocytes or red blood cells (RBCs). We introduced isotope-enriched α-synuclein into RBCs and monitored person-specific NMR signals from α-synuclein at residue-specific resolution. By analyzing the chemical shifts and line broadening of α-synuclein, as well as the pattern of post-translational modifications, we probed the environment inside RBCs. To evaluate the diagnostic potential of NMR, we compared the NMR signals of α-synuclein in RBCs derived from patients with neurodegenerative disorders and the control group. In conclusion, we have successfully performed the first In-RBC NMR and demonstrated its potential for medical diagnosis.

Symposium : **PHYS3-3**

Recent Advances in Physical Chemistry for Energy Science

Room 208+209+210 FRI 15:10

Chair: Myeongkee Park (Pukyong National University)

Generation of long-lived charges in organic photoanodes with a polymer overalyer for efficient photoelectrochemical performance

Tack Ho Lee

Department of Chemistry Education, Pusan National University, Korea

Organic photovoltaic devices employing bulk heterojunctions (BHJs) of polymer donors and small molecular nonfullerene acceptors have recently demonstrated high performance, with strong visible and near-infrared absorption and low energy losses. Such junctions are promising candidates for solar-driven water splitting. Here, we investigate the role of a PM6 polymer overlayer on the photoexcited carrier dynamics in a Y6:PM6 BHJ photoanode undergoing ascorbic acid oxidation. With the additional polymer layer, the hole lifetime is increased in the solid state BHJ film. When the photoanode is electrically coupled to a hydrogen-evolving platinum cathode, hole polaron states are observed on the timescale of seconds under operational conditions. More importantly, we demonstrate that the organic photoanode with the polymer overlayer shows enhanced performance, reaching over 6 mA cm^{-2} at 1.23 V_{RHE} without a co-catalyst. An EQE of 18% was observed using 850 nm excitation. We propose that the use of an organic overlayer can be an effective design strategy for generating longer charge carrier lifetimes in organic photoanodes for efficient oxidation catalysis.

Symposium : **PHYS3-4**

Recent Advances in Physical Chemistry for Energy Science

Room 208+209+210 FRI 15:30

Chair: Myeongkee Park (Pukyong National University)

Modulating Solvation Structure of Electrolytes for Lithium Metal Batteries

Kyung-koo Lee

Department of Chemistry, Kunsan National University, Korea

Even though lithium metal batteries (LMBs) have been studied since the 1970s, they have not been commercialized due to the uncontrolled growth of lithium dendrites. Effective strategies to suppress the formation of lithium dendrite have focused on increasing the solid electrolyte interface (SEI) layer stability by modifying its chemical composition.Given that the primary solvation sheath in the electrolyte serves as the precursor of solid electrolyte interphase, the interfacial chemistry on the electrodes is closely correlated to the solvation structure of electrolytes. In the case of conventional dilute electrolytes where the Li ions are usually solvated by strongly solvating polar solvents and most anions are excluded from the solvation sheath, the SEI layer is mainly composed of organic species originated from the solvent molecules. One type of unconventional electrolytes is the concept of highly concentrated electrolytes (HCEs), with high salt concentration. In HCEs, anions inevitably appear in the primary solvation sheath of Li+ to form ion pairs or aggregates because of the scarcity of solvents and abundance of anions. Another type of unconventional electrolyte is the weakly solvating electrolytes (WSEs) which contain the solvents with low dielectric constants. The limited solvating power of these solvents strengthens the electrostatic interactions between ions, resulting in a high prevalence of associated complexes even at moderate concentrations. Such distinctive solvation structures in HCEs or WSEs contribute to the formation of an anion-derived SEI, suppressing lithium dendrite formation.In this talk, examples of HCEs and WSEs will be presented, elucidating the correlation between molecular properties and solvation structures within the electrolyte system.

Symposium : **PHYS3-5**
Recent Advances in Physical Chemistry for Energy Science
Room 208+209+210 FRI 15:50
Chair: Myeongkee Park (Pukyong National University)

Control of Excitonic Behaviors in Semiconductor Nanocrystals for Light Harvesting and Light Amplification Applications

Jiwon Bang

Incheon National University, Korea

Exciton in colloidal semiconductor nanocrystals is unique in many ways in comparison with the excited states of either molecular species or bulk materials, and colloidal semiconductor nanocrystals have garnered significant attention in the realm of light harvesting and emission materials. However, the strong Coulombic interaction of tightly bound electron-hole pairs within three-dimensional confined structure poses considerable challenges in the manipulation of excitonic behaviors, thereby impeding advancements in applications related to light harvesting and amplification. To overcome these challenges, we have undertaken a concerted effort to modulate carrier distribution within thee nanostructures characterized. This modulation is achieved through strategies involving doping or precise control of morphology, aimed at optimizing the utilization of charge carriers in their excited states with suppressing undesired dissipation processes. Notably, the incorporation of transition metal ions within II-VI or III-V nanomaterials serves to localize the charge carriers, thereby diminishing electron-hole interactions and facilitating an enhancement in charge extraction efficiency. Additionally, manipulation of the spatial distribution of charge carriers within QDs has been achieved through precise control over the internal architecture of CdSe/CdS core/shell quantum dot configurations, and these engineered nanomaterials exhibit amplified emission characteristics under nanosecond optical excitation conditions. The characterization of these materials has been conducted through the time-resolved spectroscopic analysis, thereby affording insights into exciton behaviors within the strong confinement regime.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **PHYS3-6**
Recent Advances in Physical Chemistry for Energy Science
Room 208+209+210 FRI 16:10
Chair: Myeongkee Park (Pukyong National University)

C1 conversions over well-defined model surfaces probed with ambient pressure X-ray photoemission spectroscopy

Jeongjin Kim

Pohang Accelerator Laboratory, Korea

The sustainable utilization technology for carbon dioxide (CO2) still has many drawbacks of CO2 activation under mild conditions in industrial processes because of the high activation energy barrier of CO2. In surface science, we have focused on the revealing CO2 activation process over well-defined model catalysts, considering the issues of pressure and material gaps. One of the emerging characterization techniques, ambient pressure X-ray photoelectron spectroscopy (AP-XPS), is unveiling the momentous reaction steps of CO2 dissociation and sequentially formed intermediate species at the gas-solid interface. The probed chemical bonding or binding information provides critical evidence for understanding CO2 activation towards value-added chemicals at the molecular level. In this talk, I will discuss in situ surface catalysis studies on the conversion of light carbon (C1) molecules into methane or methanol. Particularly, I will highlight the physical behavior of nickel (Ni)- or copper (Cu)-based metal-oxide catalysts for facile carbon diffusion and transfer at the interface. The modified surface geometries and electronic states by surface alloy formations may induce facile molecular conversions for the dissipation of hydrogen or coupling of carbon-terminated intermediates. The synchrotron-based AP-XPS technique can resolve the difference in chemical binding species of molecularly adsorbed CO2 and dissociated adsorbates by the cleavage of O=C=O bonds at ambient pressures. In addition, the characteristic electron transitions among X-ray absorption edges could give us useful information to interpret unusual catalytic processes. Those systematic in situ observations will shed light on the novel catalyst design and advances in energy science.

Award Lecture in Division : **ANAL1-5**
Recent Trends in Analytical Chemistry Research for Industrial Applications
Room 214 THU 17:00
Chair: Sang Yun Han (Gachon University)

Magnetoplasmonics-based Chiral Biomedical Sensing for Point Mutation of DNA

Jaebeom Lee

Chemistry, Chungnam National University, Korea

Hereditary hearing loss households have identified several genetic mutations and their preemptive diagnosis through fetal DNA detection is crucial to prevent further deteriation of hearing loss. In this paper, the clinical validity of chiral detection experiments for monitoring DNA point mutations has been demonstrated using Ag@Fe3O4 magnetoplasmonic nanoparticles (MagPlas NPs) and their plasmonic nematic films (PNFs). First, we show in-depth study of chiroptical property in the PNFs and symmetric breaking mechanism by Au NPs conjugated with DNA, which is associated with hereditary non-syndromic hearing impairment (HNSHI). As a results, attendance of the HNSHI-related DNA with point mutation could be detected in PNF system, which can produce unique chiral signals up to 10 -18 mol. Magnetic circular dichroism (MCD) study was accomplished to understand light and matter interaction under the designated field, which tells us apparent mechanism of CD signal enhancing. It is probable that the developed sensing system is eventually helpful to pre-natal clinical gene diagnosis and treatment.

Symposium : **ANAL1-1**

Recent Trends in Analytical Chemistry Research for Industrial Applications

Room 214 THU 15:40

Chair: Kihun Kim (KIST)

Recent Trends in Point-of-Care Testing for Infectious Diseases

Jaebum Choo

Department of Chemistry, Chung-Ang University, Korea

Over the past three years, coronavirus disease 2019 (COVID-19) has resulted in unprecedented widespread casualties worldwide. Despite declaring an end to the global health emergency phase of COVID-19, the threat of post-pandemic infectious diseases still remains. Respiratory infections like COVID-19 can be transmitted through the air, underscoring the importance of swiftly and accurately diagnosing confirmed cases and isolating individuals. Hence, there is an immediate need to develop innovative point-of-care testing (POCT) techniques capable of swiftly and accurately diagnosing infectious diseases on-site. In this presentation, I will briefly explore the underlying principles and constraints of currently available *in vitro* diagnostic devices and introduce emerging POCT systems to prepare for future pandemics.

Symposium : **ANAL1-2**

Recent Trends in Analytical Chemistry Research for Industrial Applications

Room 214 THU 16:00

Chair: Kihun Kim (KIST)

Determination of Fe_3O_4 concentration in sintered ores using Raman spectroscopy and image analysis

Hoeil Chung

Department of Chemistry, Hanyang University, Korea

Raman measurement scheme designed for the determination of Fe_3O_4 concentration in sintered ores, highly photon-absorbing brownish black samples, was demonstrated. Initially, to prevent sample burning, the laser power per area was decreased by widening laser illumination diameter to 1 mm for spectral acquisition. In addition, to further increase the intensity of Fe_3O_4 peak without thermal oxidation, the water-wetting of sintered ore sample was accomplished to lessen the laser-driven sample heating. With the determined measurement settings, Raman spectra of all the real 100 sintered ore samples were collected. The correlation between the Fe_3O_4 concentration determined by a conventional titration method and ratio of Fe_3O_4 and Fe_2O_3 peak areas was good with R^2 of 0.92. Moreover, since the color of sintered ore would be representative of the relative abundance of the constituents, a simple color analysis of the sample (no Raman measurement) was attempted as an alternative to determine the Fe_3O_4 concentrations. The results in both cases were comparatively discussed.

Symposium : **ANAL1-3**

Recent Trends in Analytical Chemistry Research for Industrial Applications

Room 214 THU 16:20

Chair: Kihun Kim (KIST)

MILPIG: Metabolic Isotope Labeling of Glycans

Jae-Min Lim

Department of Chemistry, Changwon National University, Korea

Changes in glycan expression affect many biological functions of glycoproteins and induce physiological changes. To understand the biological relevance of glycans, many mass spectrometry (MS)-based methods have been developed for the relative quantification of glycans using stable isotopic labeling. To understand the biological relevance of glycans, based on duplex MILPIG (metabolic isotope labeling of polysaccharides with isotopic glucose), we establish here a novel triplex isotope labeling method using baker's yeast as a model system. Two differentially isotope-labeled glucoses (medium: 1-13C1 and heavy: 1,2-13C2), in addition to natural abundance glucose (light), were successfully used to label each sugar ring in N-linked glycans in three different cell culture conditions, resulting in a predictable triplet spectrum that is amenable for relative quantitation. The absolute area of the triplet signals was calculated at a 1:1:1 mixing ratio of the glycans to evaluate comparative quantification and reproducibility. The area ratios among the triplet peaks were within 3.3% of the expected, with standard deviation was 0.08, indicating excellent relative quantitative performance.In addition to N-linked glycans, we also obtained isotope-labeled O-linked glycans from the MILPIG method without mass spectral interference for O-linked glycans with a small number of sugars. In the yeast model system incubated with pyruvate and glucose, respectively, relative quantitative results were obtained in which the expression of O-linked glycans was doubled in pyruvate.

Symposium : **ANAL1-4**

Recent Trends in Analytical Chemistry Research for Industrial Applications

Room 214 THU 16:40

Chair: Kihun Kim (KIST)

Advanced TEM as the Key to Deciphering Structure-Property Relationships in Functional Organic Materials

Eunji Lee

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

In the evolving field of materials science, unlocking the potential of organic and polymer materials drives cross-industry innovation. As we strive to maximize their potential, a central challenge arises: deciphering the interplay between structure and properties. Recent trends highlight the need for precision in bridging this gap, especially amidst increasing material diversity driven by rapid industrial innovation. Advanced Transmission Electron Microscopy (TEM) emerges as an insight beacon within this context, offering direct analysis of functional nanomaterials' evolving landscape. Here, we review the pivotal role of advanced TEM in guiding the synthesis and understanding of functional organic materials, highlighting the importance of recent advances in TEM as a navigation tool for property improvement. From 3D assemblies of organic semiconductors ready to reconfigure flexible electronics to the implications of the nanoscale morphology of polymer blends for energy storage, we demonstrate the power of TEM to visualise the invisible. Our explorations are dynamically extended by in situ TEM studies that capture changes in materials in response to external stimuli, similar to the time-lapse evolution of nature. We explore the impact of AI and machine learning on automating the analysis of complex TEM data. The trajectory of advanced TEM involves the convergence of many disciplines, including nanotechnology, materials science, and analytical chemistry. We highlight the importance of TEM in reframing the view of functional nanomaterials in organic materials design and engineering.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ANAL2-1**
Recent Trends in Advanced Analytical Chemistry
Room 214 FRI 14:30
Chair: Min-Sik Kim (DGIST)

Elevating Biosensor Performance through Signal Amplification Strategies

Hee Kyung Na

Bio-imaging team, Korea Research Institute of Standards and Science, Korea

The pursuit of highly sensitive biosensors for detecting low-abundance biomarkers has fueled the development of advanced signal amplification strategies. This presentation underscores the importance of signal amplification techniques in biosensor research, particularly in the context of enhancing sensitivity and reproducibility for biomarker detection. Focusing on Localized Surface Plasmon Resonance (LSPR), Mass Spectrometry (MS), and Surface-Enhanced Raman Spectroscopy (SERS) sensors, we present novel strategies for signal enhancement. This research leads to synergistic approaches that promise transformative advances in biosensing capabilities, spanning medical, environmental, and research applications.

Symposium : **ANAL2-2**

Recent Trends in Advanced Analytical Chemistry

Room 214 FRI 14:50

Chair: Min-Sik Kim (DGIST)

Single-molecule Optical Nanoimmunosensors for Supersensitive Detection

Seungah Lee

Department of Applied Chemistry, Kyung Hee University, Korea

Single-molecule optical nanoimmunosensors are leading a revolutionary development in biosensing and enabling ultra-sensitive detection of biological molecules. We developed a method based on optical nanotechnology for detecting biomolecules at the single-molecule level, and reported the groundbreaking achievements for the detection of trace amounts of biological molecules. Single-molecule optical nanoimmunosensors detected the antibody-antigen interactions at the single-molecule level, allowing to identify important biological molecules, such as markers of serious disease, at the zeptomolar level. In addition, we demonstrated that nanoscale optical sensing can be utilized for reliable and accurate detection even in complex biological samples. This research provides an important foundation for the development of future ultra-sensitive biosensing technologies and will open up innovative opportunities in a variety of applications requiring accurate and rapid detection of biological molecules.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **ANAL2-3**
Recent Trends in Advanced Analytical Chemistry
Room 214 FRI 15:10
Chair: Min-Sik Kim (DGIST)

Nanostructure-based laser desorption/ionization time-of-flight mass spectrometry for analysis of various small molecules

Young-Kwan Kim

Department of Chemistry, Dongguk University, Korea

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) is one of the most powerful soft-ionization techniques. Therefore, MALDI-TOF-MS has been extensively harnessed for mass spectrometric analysis of high-molecular weight compounds such as proteins, nucleic acids, and synthetic polymers owing to its high resolution and sensitivity. Despite those advantages, it has been not applicable to analysis of low-molecular weight compounds (m/z

Symposium : **ANAL2-4**

Recent Trends in Advanced Analytical Chemistry

Room 214 FRI 15:50

Chair: Min-Sik Kim (DGIST)

Step-efficient Design and Bioanalytical Characterization of Selective Metal Binding Proteins

Tae Su Choi

Division of Life Sciences, Korea University, Korea

In this talk, I will introduce design approaches for artificial metalloproteins using flexible protein scaffolds and discuss the biochemical lessons that can be learned from designed proteins. Metalloproteins are closely associated with vital functions of living organisms, such as metal homeostasis and enzymatic reactions. Central to the functions of metalloproteins is selective metal coordination; each metalloprotein must pair with its cognate metallocofactor to fulfill its biological role. Without the aid of intracellular regulatory mechanisms, most metalloproteins in heterogeneous environments exhibit low fidelity in metal selectivity. Inherently flexible motions of protein backbones and side chains can disrupt steric selection of the metal ions whose d-orbital electron configurations determine preferred coordination geometries. Accordingly, a large number of metalloproteins have been reported to generally follow the Irving-Williams (IW) series (MnII < FeII < CoII < NiII < CuII > ZnII) in binding affinities between the metal ions and the proteins, thereby losing their intrinsic structural/catalytic functionalities. I will discuss the design strategy and characterization of artificial dimeric proteins that thermodynamically overcome the IW restrictions in vitro and in cellulo, favoring the binding of lower-IW transition metals over CuII - the most dominant ion in the IW series. Additionally, I will also present how the flexible dimer scaffold could be systematically applied to new variants with different metal selectivity or enzymatic activity.

Symposium : **ANAL2-5**
Recent Trends in Advanced Analytical Chemistry
Room 214 FRI 16:10
Chair: Min-Sik Kim (DGIST)

Enhancement of solution NMR sensitivity and resolution for studying various biomolecules: exploiting the media for labile protons

Jihyun Kim

Chemistry Education, Kyungpook National University, Korea

Nuclear Magnetic Resonance (NMR) has long been used for identifying structures and dynamics of various biomolecules, including proteins, DNAs, and RNAs, due to its ability to characterize these properties at an atomic-resolution level. However, a limitation of this technique is the low sensitivity of NMR signals, which demands a long experimental time with signal averaging. Further, detecting labile proton signals on biomolecules such as NH or OH is challenging not only due to this intrinsic low NMR sensitivity but also due to the exchange of labile hydrogens with solvent protons, leading to signal loss. This problem sometimes causes difficulties in the determination of biomolecule structures, as labile protons contain key information about their structure. In this presentation, we will introduce new NMR methods utilizing the solvent exchange phenomena to increase the sensitivity of ^{1}H NMR experiments. These new methods are combined with multidimensional and multiplexing schemes to improve efficiency and resolution. The applications of these experiments are demonstrated on RNA fragments derived from the SARS-CoV-2 virus and intrinsically disordered proteins.

Symposium : **LIFE1-1**
Recent Advances in Biomolecular Condensation
Room 304+305+306 THU 15:40
Chair: Jongmin Park (Kangwon National University)

Controlled synthesis of phase separated protein condensates

Yongwon Jung

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

Phase separation of specific biomolecules into liquid droplet-like condensates (process called liquid-liquid phase separation, LLPS) is a key mechanism to form membrane-less organelles, which spatio-temporally organize diverse biochemical processes in cells. At the same time, these liquidic protein condensates also offer new and highly attractive biomaterials that can contain specific sets of biomolecules with extremely high densities and dynamic liquid properties. However, ways to manipulate protein condensate materials remain largely unexplored. For more precise manipulation of these condensates, it is critical to have diverse but simplified model systems. Our group have been developing various protein-based in vitro LLPS models, and used these models to control/produce diverse condensate materials with intended sizes and properties. In this talk, I want to introduce our recently developed strategies to fabricate functional and structurally precise artificial protein condensate-based materials.

Symposium : **LIFE1-2**

Recent Advances in Biomolecular Condensation

Room 304+305+306 THU 16:10

Chair: Jongmin Park (Kangwon National University)

Biomolecular Phase Separation and Preferential Binding

Jeong-Mo Choi

Department of Chemistry, Pusan National University, Korea

In the past decade, there has been a growing interest in the phase behavior of biomolecules, especially following the demonstration of its biological implications, such as the reversible formation and dissociation of biomolecular condensates. These condensates can play a wide range of crucial functions inside cells, and one of them is accelerating chemical reactions. There is a burgeoning interest in uncovering the underlying principles and leveraging them as tools in synthetic biology to engineer cellular systems.While the initial notion suggested that the acceleration of reactions within condensates was solely due to the elevated concentration of functional molecules, recent research has revealed that other factors also contribute to this acceleration. In this presentation, I will introduce the polyphasic linkage model, which posits the preferential binding of ligands to one of two distinct phases that arise during phase separation. To illustrate the model's applicability, I will demonstrate its ability to effectively explain in-cell phase separation driven by a protein called gephyrin.

Symposium : **LIFE1-3**

Recent Advances in Biomolecular Condensation

Room 304+305+306 THU 16:40

Chair: Jongmin Park (Kangwon National University)

Integrating light and temperature information by biomolecular condensates in plants

Jae-Hoon Jung

Department of Biological Sciences, Sungkyunkwan University, Korea

Plant constantly adjust their growth and development in response to their environments to maximize fitness and reproductive success. Temperature is one of the most influential environmental factors controlling plant fitness as it affects the rate of every physicochemical reaction. Prolonged exposure to warm temperatures triggers a set of developmental responses that are collectively referred to as thermomorphogenesis: plants exhibit increased elongation growth of the hypocotyl and primary root as well as accelerated flowering and seed set at warm temperatures. Temperature cues are not perceived in isolation but are integrated with a variety of other environmental and endogenous signals. In Arabidopsis, light and temperature sensing are particularly intertwined. How are light and temperature information spatially and temporally integrated? Recent research on liquid-liquid phase separation indicates that microenvironments within biomolecular condensates confer spatial and temporal specificity to light and temperature responses. In this talk, I will briefly summarize recent studies on the role of biomolecular condensates in light and temperature sensing and discuss how light and temperature signals interact via the formation of biomolecular condensates in plants.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **LIFE1-4**

Recent Advances in Biomolecular Condensation

Room 304+305+306 THU 17:10

Chair: Jongmin Park (Kangwon National University)

Capturing intranuclear topology of subnuclear condensates relative to transcription

Won-Ki Cho

Department of Biological Science, KAIST, Korea

Mammalian genome is organized into a hierarchical structure at multiple scales in a cell nucleus. Recent intensive studies using live-cell imaging techniques have characterized behaviors of subnuclear compartments, exemplified with transcriptional condensates and nuclear speckles. They are functionally specialized non-membrane bound organelles, mostly follow liquid properties. However, how the genome structure and subnuclear organelles are spatially organized in the nucleus has not been elucidated. We found that chromatin looping by CTCF, a chromatin architectural protein, acts as an architectural prerequisite for the assembly of phase-separated transcriptional condensates. Moreover, we observed a layered structure of transcriptional and splicing condensates near the nuclear matrix discovered by super-resolution imaging of RNA polymerase II, nuclear speckles, and Scaffold attachment factor A (SAF-A, a nuclear matrix associated proteins).

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **LIFE2-1**
Recent Advances in Biosystems Engineering
Room 305+306 FRI 09:00
Chair: Minseob Koh (Pusan Natioanl University)

Enzyme engineering with non-canonical amino acid

Hyungdon Yun

Department of Systems Biotechnology, Konkuk University, Korea

Protein engineering techniques such as rational design and directed evolution have found widespread applications in improving or altering the intrinsic activities of numerous enzymes. However, these strategies are primarily based on nature's alphabet of twenty canonical amino acids (cAAs). A series of orthogonal amino-acyl transfer RNA (tRNA) synthetase (aaRS)/tRNA pairs have been developed to encode distinct non-canonical amino acids (ncAAs) in vivo. Over the last two decades, more than 200 ncAAs have been genetically encoded in prokaryotes and eukaryotes. Apart from peptide modification and antibody development for pharmaceutical use, ncAAs have been widely applied in enzyme engineering research to illustrate the enzyme mechanisms, enhance enzyme activity, and even generate new catalytic mechanisms into protein scaffolds. Although progress in this field is fast, only a handful of examples have been reported for remodeling enzyme active sites by introducing single ncAA resulting in improved activity and substrate scope compared to cAAs. Here, I will introduce our recent efforts to engineer enzyme with ncAA for enhancing the functionality of enzymes.

Symposium : **LIFE2-2**

Recent Advances in Biosystems Engineering

Room 305+306 FRI 09:30

Chair: Minseob Koh (Pusan Natioanl University)

Development of new biocatalysts for plastic biodegradation and their potential biochemical pathway

Soo-Jin Yeom

School of Biological Sciences and Technology, Chonnam National University, Korea

Plastic contamination currently threatens a wide variety of ecosystems and presents damaging repercussions and negative consequences for many wildlife species. Sustainable plastic waste management is an important approach to environmental protection and a necessity in the current life cycle of plastics. In this regard, plastic biodegradation by microorganism is most notable. The decomposition of polyethylene (PE), an extremely recalcitrant synthetic polymer, using microorganisms is an ideal and sustainable method for PE bio-treatment in the future. We isolated a set of PE-biodegrading Bacillus species from a landfill site. Among them, Bacillus thuringiensis JNU01 exhibited the highest cell growth rate in PE media, which means it effectively decomposed PE to use in the metabolic pathway as a sole carbon source. B. thuringiensis JNU01-treated PE showed new chemical functional groups such as hydroxyl, carboxyl, and amide groups in the inert hydrocarbon. Scanning electron microscopy revealed considerable physical damage on the surface of the PE film after treatment with B. thuringiensis JNU01. Furthermore, various alkane derivatives obtained from PE were characterized using gas chromatography-mass spectrometry. On the other hand, increase of the mRNA transcriptional levels of B. thuringiensis JNU01 strain in the presence of PE suggests that an CYP102A5 variant (CYP102A5.v1) involve for PE biodegradation. Finally, we confirmed that purified CYP102A5.v1 catalyzes the hydroxylation reaction of PE by NADPH oxidation assay and FT-IR analysis. These results show that B. thuringiensis JNU01 is a potential PE decomposer and suggest that CYP102A5.v1 can be a trigger biocatalyst to hydroxylate PE.


H H
C C
H H n
Polyethylene
Bacillus thuringiensis JNU01

Symposium : **LIFE2-3**

Recent Advances in Biosystems Engineering

Room 305+306 FRI 10:00

Chair: Minseob Koh (Pusan Natioanl University)

To build and visualize chromatin: Engineering the epigenome

Minhee Park

Korea Advanced Institute of Science and Technology (KAIST), Korea

Epigenetic regulation allows genetically identical cells to generate distinct gene expressions and phenotypic states that persist during cell division. The repurposing of epigenetic regulation offers great opportunities for the development of next-generation cellular control. While the engineering of epigenetic regulation is promising, it remains challenging due to the lack of identifiable parts and components sufficient for epigenetic behaviors.

We apply a bottom-up synthetic biology approach to develop a minimal synthetic epigenetic system based on the principle of classic "read-write" motif. We exploit DNA adenine methylation (6mA), a DNA modification that is rarely found in metazoan genomes, to create a fully synthetic chromatin system in human cells. Together with a quantitative model of chromatin dynamics, we show these circuits mediate the spreading of the modification to regulate genes at a distance and the establishment of long-term epigenetic memory, demonstrating the sufficiency of the read-write mechanism for epigenetic memory. We also explore additional motifs governing epigenetic regulation, one of which is the 3D chromatin structure. We combine user-defined synthetic control of epigenetic silencing and super-resolution 3D chromatin imaging to quantitatively delineate 3D chromatin organization and epigenetic memory mechanisms at single-nucleus resolution.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **LIFE2-4**
Recent Advances in Biosystems Engineering
Room 305+306 FRI 10:30
Chair: Minseob Koh (Pusan Natioanl University)

Click chemistry-mediated engineering of therapeutic proteins & in vivo imaging

Inchan Kwon

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

Therapeutic proteins play an important role in curing various human diseases. Therapeutic proteins administered to patients are constantly eliminated from the blood via several mechanisms including renal filtration, proteolytic degradation, and intracellular degradation. Therefore, therapeutic proteins should be periodically administered, leading to poor patient compliance. However, the conjugation of serum half-life extender to random sites of therapeutic protein led to a significant loss of therapeutic activity. Therefore, our research group has been exploring site-specific conjugation of human serum albumin (HSA) to therapeutic proteins to extend the serum half-life. First, a non-natural amino acid with a click chemistry handle was site-specifically introduced to a therapeutic protein without compromising the therapeutic activity. In order to increase the conjugation yield of HSA to therapeutic proteins, we developed the engineered orthogonal pair recognizing a non-natural amino acid with a tetrazine functional group, allowing very fast bioconjugation through inverse electron demand Diels-Alder reaction (IEDDA). Then, human serum albumin was conjugated to the specific site. Using the very fast bioconjugation through IEDDA, we also demonstrated the efficient in vivo bioconjugation, leading to the convenient tumor imaging.


사단법인 대한화학회
KOREAN CHEMICAL SOCIETY

Award Lecture in Division : **ORGN1-1**
International Organic Chemists Symposium
Convention Hall 2 THU 15:40
Chair: Sungwoo Hong (KAIST)

Intracellular polymerization and self-assembly to control cellular fate

Ja-Hyoung Ryu

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

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

Symposium : **ORGN1-2**
International Organic Chemists Symposium
Convention Hall 2 THU 16:10
Chair: Hong Geun Lee (Seoul National University)

Visible Light-driven N-Radical Synthetic Chemistry

Jia-Rong Chen

College of Chemistry, Central China Normal University, China

Nitrogen-centered radicals (NCRs) have long been considered as a versatile class of intermediates for C−N bond formation because of their unique properties and high reactivity. Despite their power, the progress of NCR chemistry is still slow compared with the popularity of carbon-centered radicals, and their considerable synthetic potential has been largely unexplored.

Building on the unique activation modes of visible-light photocatalysis, over the past decade, we have developed a range of visible light-induced photoredox-catalyzed strategies for controlled generation of various NCRs under mild conditions. Employing these methods, we have developed a range of NCR-radical-based radical transformations. By merging with asymmetric metal catalysis, several types of enantioselective radical cross-coupling reactions have also been achieved. These reactions allowed construction of a wide variety of valuable nitrogen-containing compounds.

In this lecture, I will present these studies in detail with a special focus on how we have invented the reaction and expanded the mechanistic understanding.

Symposium : **ORGN1-3**

International Organic Chemists Symposium

Convention Hall 2 THU 16:45

Chair: Hong Geun Lee (Seoul National University)

New Polar and Radical Methods for the Formation of Carbon-Phosphorus Bonds : A Mechanistically-Driven Approach

Sami Lakhdar

Laboratoire Hétérochimie Fondamentale et Appliquée, CNRS, Université Paul Sabatier, France

Organophosphorus compounds are important scaffolds that have gained tremendous attention owing to their prevalence in various areas ranging from agriculture to medicine. Although there are many effective synthetic methods for forming carbon-phosphorus bonds, some of them are prone to the use of harsh reaction conditions.

The lecture will cover recent developments from our group that aim to provide practically simple methods for synthesising organophosphorus scaffolds from readily available phosphorus sources. It will also underline the importance of physical organic tools in understanding the reaction mechanisms and the design of new transformations

Symposium : **ORGN1-4**

International Organic Chemists Symposium

Convention Hall 2 THU 17:20

Chair: Hong Geun Lee (Seoul National University)

Asymmetric Catalysis with Organoboron Reagents

James P. Morken

Department of Chemistry, Boston College, United States

Chiral organoboronic esters are versatile intermediates for chemical synthesis. Not only are these compounds stable under a variety of reaction conditions, they are generally non-toxic and can be transformed with minimal generation of hazardous waste. An important feature of aliphatic organoboronic esters is that the boron atom may be replaced with an array of different functional groups through efficient, stereospecific transformations. This seminar will cover new strategies for the construction of alkylboronic esters from simple starting materials in a catalytic enantioselective fashion, and will also discuss ways in which these compounds can be used to address compelling problems in chemical synthesis.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **ORGN2-1**
Recent Trends in Organic Chemistry
Convention Hall 2 FRI 09:30
Chair: Juyoung Yoon (Ewha Womans University)

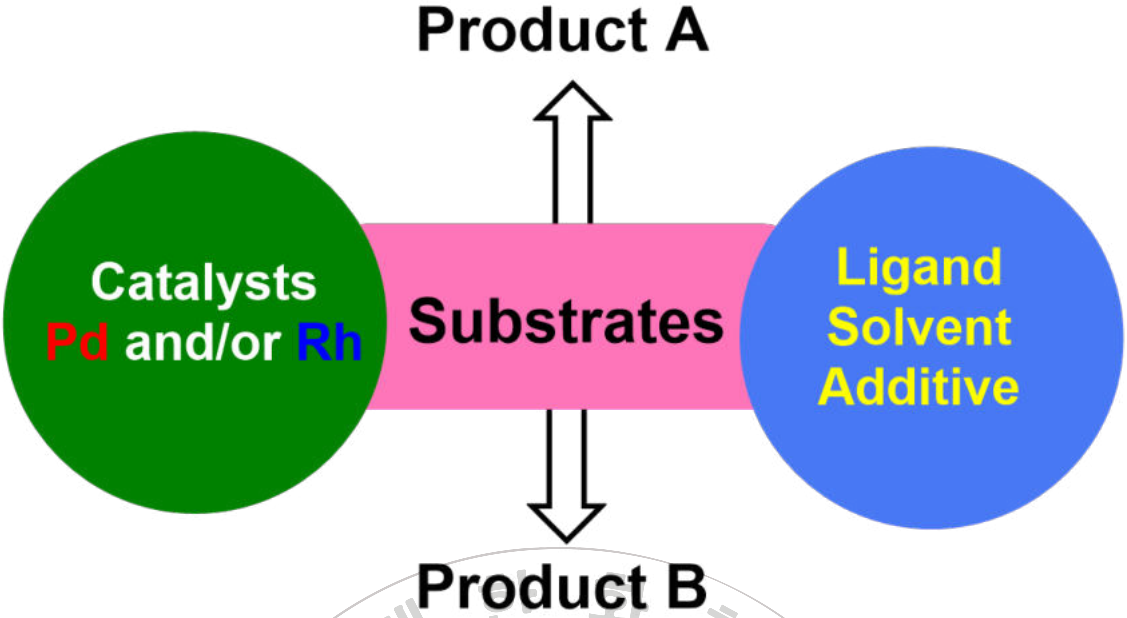
Development of Divergent Catalysis

Sang-gi Lee

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

The term ‘divergent catalysis’ describes different catalytic reactions that occur with the same substrates (reactants) under controllable conditions, which can provide different products through intricate yet precise control of different catalytic pathways. Over the past 30 years, remarkable progress in the field of asymmetric catalysis could allow to provide both enantiomers (enantiodivergent catalysis) mostly by using enantiomeric chiral ligands. However, the examples of rationally designed diastereo-, regio-, and chemodivergent catalysis are still few. In this seminar, our recent studies on novel divergent catalytic reactions using Pd and/or Rh catalysts will be presented; examples include tandem divergent transformations of Blaise reaction intermediates,[1] tandem divergent cyclopropanations through solvent-driven regioselective $C(sp^3)$-H bond activation,[2] divergent intramolecular transformations of *N*-sulfonyl-1,2,3-triazoles,[3] divergent asymmetric spiroannulations,[4] catalyst-controlled divergent $C(sp^3)$-H/C_{Ar}-H bond functionalizations of α-diazoacetamides.[5]

Reference
[1] Kim, J. H. et al. *Angew. Chem. Int. Ed.* **2014**, *53*, 6435.
[2] Chung, D.S. et al. *Angew. Chem. Int. Ed.* **2018**, *57*, 15460.
[3] (a) Ko, Y. O. et al. *Org. Lett.* **2016**, *18*, 6432. (b) Lee, K. R. et al. *Org. Biomol. Chem.* **2021**, *19*, 5093.
[4] Jeon, H. J. et al. *Org. Lett.* **2022**, *24*, 9189.
[5] (a) Huang, L.-Z. et al. *ACS Catal.* **2018**, *8*, 7340. (b) Lee, Y. L. et al. **2023**, under revision


Product A
Catalysts
Pd and/or Rh
Substrates
Ligand
Solvent
Additive
Product B

Symposium : **ORGN2-2**

Recent Trends in Organic Chemistry

Convention Hall 2 FRI 09:55

Chair: Juyoung Yoon (Ewha Womans University)

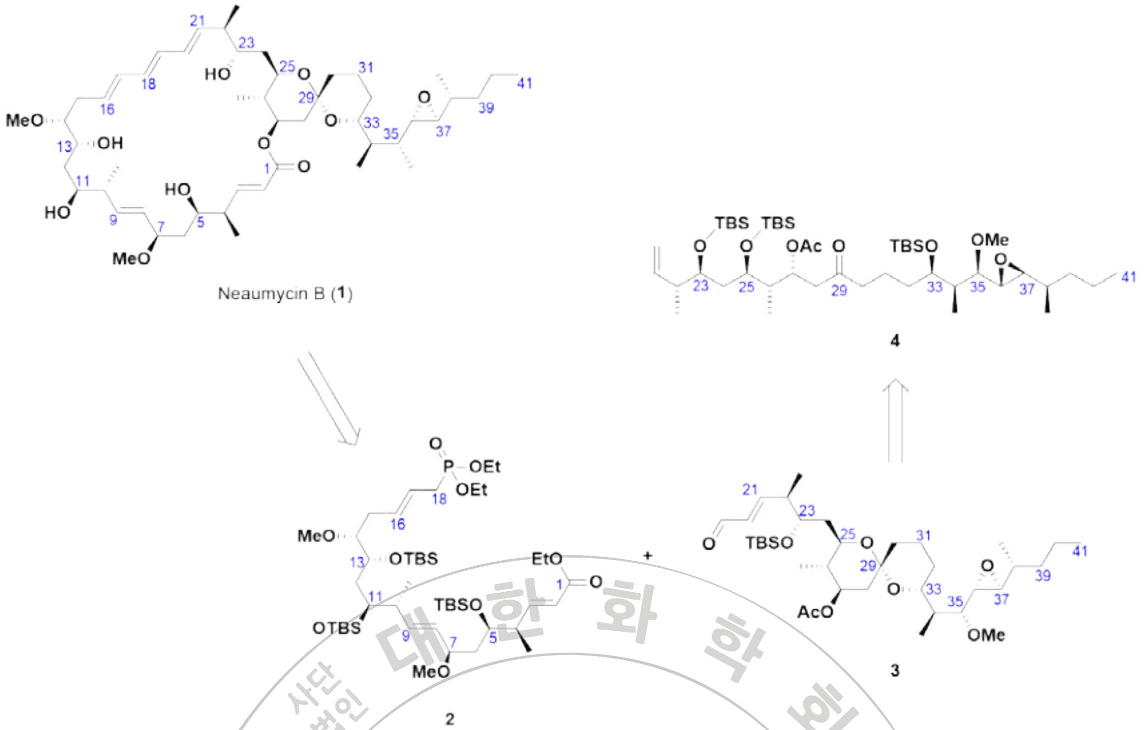
Efforts Towards the Synthesis of Neaumycin B

Suin Cho, Eungyeong Choi[1], Duck-Hyung Lee[1,*]

Sogang University, Korea

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

A group of Neaumycins was initially isolated in 2012 from the soil-dwelling microorganism Steptomyces sp. NEAU-x211. Neaumycin B (1), a 28-membered macrolide compound with 19-chiral centers and 6,6-spiroketal structure, has demonstrated significant efficacy and selectivity against U87 human glioblastoma in addition to the NCI 60 cell lines. Herein, we present our efforts toward the stereoselective synthesis of neaumycin B (1). The C1-C18 fragment (2) was prepared using Brown syn-crotylation, olefin metathesis, and NHK reaction as key steps and the C21-C41 fragment (4) was synthesized using Brown anti-crotylation, (S)-CBS reduction and Paterson aldol reaction as key steps. And conversion of the intermediate 4 into the spiroketal core of C21-C41 (3) would be pursued by acid-catalyzed cyclization and olefin metathesis of 4.


Neaumycin B (1)
4
2
3
MeO
OH
HO
MeO
HO
O
TBS
OAc
TBSO
OMe
P
OEt
OTBS
EtO
AcO
+

Symposium : **ORGN2-3**
Recent Trends in Organic Chemistry
Convention Hall 2 FRI 10:20
Chair: Juyoung Yoon (Ewha Womans University)

B–H Functionalization of *o*-Carborane

Phil Ho Lee

Department of Chemistry, Kangwon National University, Korea

Carboranes, which are recognized as a type of three-dimensional kindred of benzene, have found a number of applications in boron neutron capture therapy (BNCT) as medication, in organometallic and coordination chemistry as novel ligands, and in supramolecular design and materials as building blocks. The distinctive structures of carboranes make their derivatization laborious, which results in a restricted application range. Therefore, it is highly required to develop new synthetic methods for the functionalization of carboranes. In general, cage boron functionalization is much more challenging than cage carbon functionalization because of not only its site-selectivity among ten cage B−H bonds over only three reactive sites in arene C−H activation but also its much lower reactivity of cage B−H over cage C−H bond. Herein, we present a variety of transition metal-catalyzed B–H functionalization of *o*-carborane such as cyclative indenylation, dienylation, allenylation, amidation, acyloxyation, diacetoxylation, acylmethylation, pyrazolization, triarylation and asymmetric alkylation.

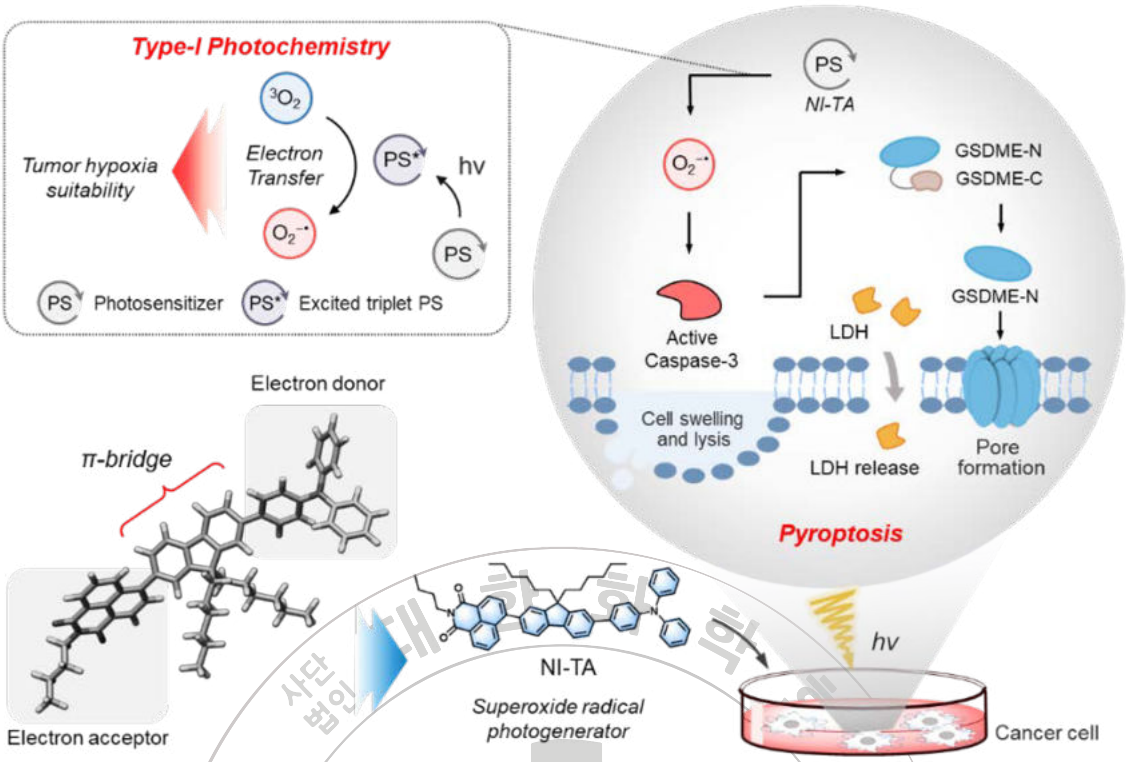
Symposium : **ORGN2-4**
Recent Trends in Organic Chemistry
Convention Hall 2 FRI 10:45
Chair: Juyoung Yoon (Ewha Womans University)

Photocatalytic superoxide radical generator that induces pyroptosis in cancer cells

Jong Seung Kim

Department of Chemistry, Korea University, Korea

Pyroptosis, a newly characterized form of immunogenic cell death, is attracting increasing attention as a promising approach to cancer immunotherapy. However, biocompatible strategies to activate pyroptosis remain rare. Here we show that a photocatalytic superoxide radical (O2−•) generator, NI-TA, triggers pyroptosis in cancer cells. NI-TA was designed to take advantage of an intramolecular triplet-ground state splitting energy modulation approach. Detailed studies revealed that the pyroptosis triggered by NI-TA under conditions of photoexcitation proceeds through a Caspase-3/gasdermin E (GSDME) pathway rather than via canonical processes involving Caspase-1/gasdermin-D (GSDMD). NI-TA was found to function via a partial O2-recycling mode of action and to trigger cell pyroptosis and provide for effective cancer cell ablation even under conditions of hypoxia (≤ 2% O2). In the case of T47D 3D multicellular spheroids, good antitumor efficiency, as well as stemness inhibition are achieved. This work highlights how photocatalytic chemistry may be leveraged to develop effective pyroptosis inducing agents



Type-I Photochemistry
$^3O_2$
Electron Transfer
PS*
hv
Tumor hypoxia suitability
$O_2^{-\bullet}$
PS
PS Photosensitizer
PS* Excited triplet PS
PS
NI-TA
$O_2^{-\bullet}$
GSDME-N
GSDME-C
GSDME-N
Active Caspase-3
LDH
Cell swelling and lysis
LDH release
Pore formation
Pyroptosis
Electron donor
π-bridge
Electron acceptor
NI-TA
Superoxide radical photogenerator
hv
Cancer cell

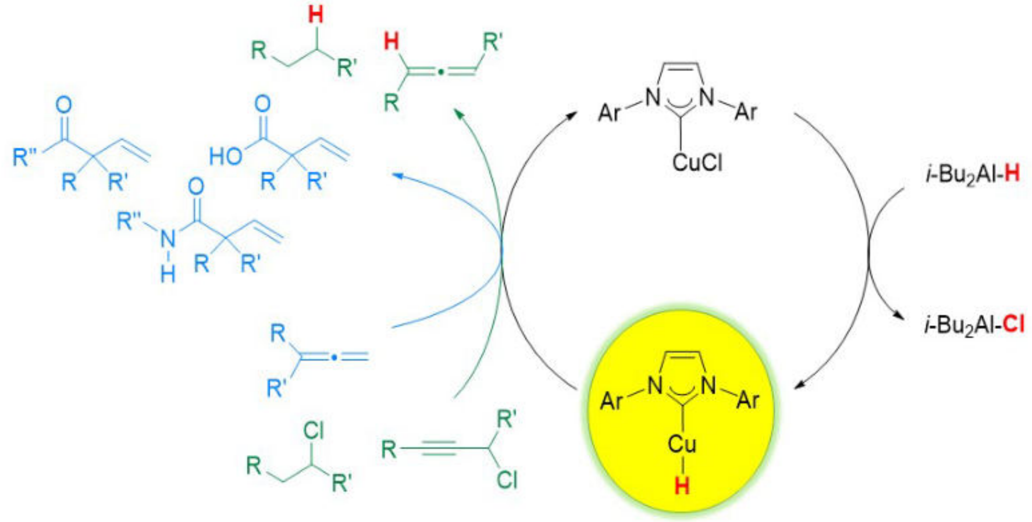
Symposium : **ORGN3-1**
Recent Trends in New Catalytic Reaction
Convention Hall 2 FRI 14:30
Chair: Han-Yong Bae (Sungkyunkwan University)

NHC-Copper Hydride Catalysis using Diisobutylaluminum Hydride

Yunmi Lee

Department of Chemistry, Kwangwoon University, Korea

Copper hydride (CuH)-catalyzed reactions have proven to be a valuable tool in the field of carbon-hydrogen bond formation. Since the pioneering work by Brunner and colleagues, who introduced the first instance of utilizing a CuH catalyst to reduce acetophenone with silanes, copper hydrides have found application in numerous catalytic transformations. While silanes and boranes stand out as common hydride sources in CuH catalysis, the utilization of aluminum hydrides in this area has received limited research attention.In this presentation, we will discuss the utilization of the readily available and inexpensive diisobutylaluminum hydride (DIBAL-H) as a new alternative source of hydride for CuH catalysis. N-Heterocyclic carbene (NHC) ligands have played a pivotal role in enhancing reactivity and controlling selectivities. Our studies have demonstrated that DIBAL-H can be effectively employed in highly regio- and stereoselective Cu-catalyzed SN2’ reductions of propargylic chlorides, enabling the synthesis of a diverse array of functionalized allenes. Furthermore, DIBAL-H has proven to be efficient for the reduction of alkyl halides. Additionally, we have developed a new approach to generate allylaluminum reagents via Cu-catalyzed hydride addition of DIBAL-H to allenes. This approach opens up new avenues for the development of unexplored allylation reactions, applying the intrinsic reactivity and Lewis acidity of aluminum.


Ar
N
N
Ar
CuCl
i-Bu2Al-H
i-Bu2Al-Cl
Ar
N
N
Ar
Cu
H
H
R
R'
H
R
R'
R''
O
R
R'
HO
O
R
R'
R''
N
H
O
R
R'
R
R'
Cl
R
R'
R
R'
Cl

Symposium : **ORGN3-2**
Recent Trends in New Catalytic Reaction
Convention Hall 2 FRI 14:55
Chair: Han-Yong Bae (Sungkyunkwan University)

Copper-Catalyzed C–C Cross-Couplings of Tertiary Alkyl Halides Enabled by Cyclopropenimine-Based Ligands

Sarah Yunmi Lee

Department of Chemistry, Yonsei University, Korea

Catalytic cross-couplings of tertiary alkyl electrophiles with carbon nucleophiles offer a powerful platform for constructing quaternary carbon centers, which are prevalent in bioactive molecules. However, these reactions remain underdeveloped, primarily by steric challenges that impede efficient bond formation. In this presentation, we describe the copper-catalyzed synthesis of such centers through the $C(sp^3)$–$C(sp^2)$ bond-forming reaction between tertiary alkyl halides and arene rings of aniline derivatives, enabled by the strategic implementation of bidentate bis(cyclopropenimine) ligands, without the aid of light or oxidants. The copper catalyst anchored by two imino-nitrogen atoms of these ligands, which have never been employed in metal catalysis previously, is highly effective in rapidly activating tertiary halides to generate alkyl radicals, allowing them to react with aryl nucleophiles under mild conditions with remarkably short reaction times (1–2 h). Various tertiary halides bearing carbonyl functional groups can be coupled with secondary or primary anilines, furnishing a range of quaternary carbon centers in good yields. Several mechanistic observations support the generation of copper(II) species and alkyl radicals which in result elucidate the steps in the proposed catalytic cycle.

Symposium : **ORGN3-3**

Recent Trends in New Catalytic Reaction

Convention Hall 2 FRI 15:20

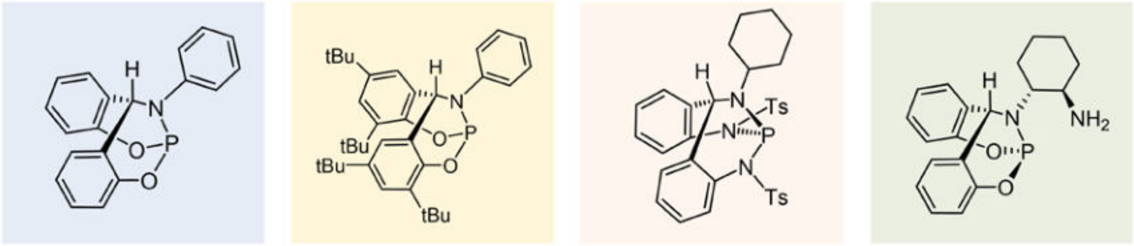
Chair: Han-Yong Bae (Sungkyunkwan University)

Ligand Control in Transition Metal Catalysis

Hyunwoo Kim

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

Transition metal catalysis has garnered significant attention due to its potential to enable novel chemical reactions and facilitate environmentally friendly processes in the pharmaceutical and fine-chemical industries. The effectiveness of transition metals as catalysts heavily relies on the properties of the ligands that interact with the central metal atoms. Consequently, the exploration of ligand effects has emerged as a prominent area of study in the realm of transition metal catalysis. To unlock new possibilities in this field, it is imperative to create a distinct category of ligands that possess distinctive electronic and structural characteristics.During this presentation, we will introduce two ligand-controlled transition metal catalytic reactions. First, we have made advancements in the field of Pd-catalyzed hydrosilylation through the development of hemilable P,O ligands. The unique hemilabile nature of these ligands is not only instrumental in achieving exceptional reactivity for the hydrosilylation of unactivated alkenes but also in controlling the regioselectivity for diene hydrosilylation. Moreover, we have achieved Cu-catalyzed enantioselective 1,4-hydropyridylation of dienes. In addition to showcasing the results of these ligand-controlled catalytic reactions, we will discuss the detailed mechanistic studies that shed light on the underlying processes. Furthermore, computational investigations have been conducted to provide deeper insights into the reaction pathways and assist in the design of efficient catalysts.



Briphos Ligand Series

Symposium : **ORGN3-4**

Recent Trends in New Catalytic Reaction

Convention Hall 2 FRI 15:45

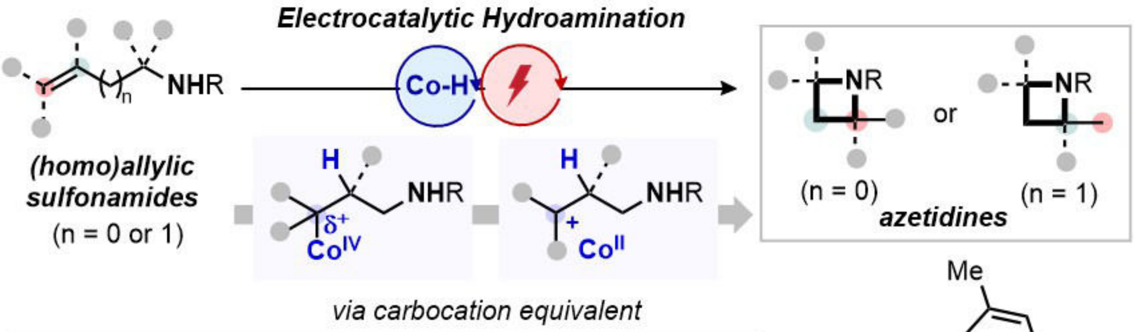
Chair: Han-Yong Bae (Sungkyunkwan University)

Cobalt-Electrocatalyzed Radical-Polar Crossover Hydrofunctionalization of Alkenes

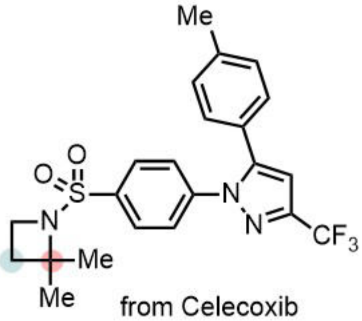
Hyunwoo Kim

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

Due to the unique reactivity of open-shell intermediates, the development of catalytic transformations driven by single-electron transfer (SET) has been an area of intense research in organic chemistry. In particular, the employment of unconventional means of activation, including photoredox catalysis and electrocatalysis, has provided unique entry to single-electron reactivities and led to new solutions to challenging synthetic problems that are not readily addressed using existing tools.We disclose a general electrocatalytic hydrofunctionalization by utilizing a wide range of alkenes. The integration of the two involves an electrochemically instigated cobalt-hydride-catalyzed radical-polar crossover of alkenes that enable the generation of key cationic intermediates, which could readily be entrapped by challenging nucleophiles. We highlight the importance of precise control of the reaction potential by electrochemistry in conjunction with the decisive role of 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) as the co-solvent to obtain optimal and exclusive chemoselectivity.In addition, we develope an electrocatalytic method for intramolecular hydroamination of allylic sulfonamides to access azetidines. The merger of cobalt catalysis and electricity enables regioselective generation of key carbocationic intermediates, which could directly undergo intramolecular C-N bond formation. The mechanistic investigations including electrochemical kinetic analysis suggest that the catalyst regeneration by nucleophilic cyclization is involved in the rate-determining step (RDS) of our electrochemical protocol and highlight the ability of electrochemistry in providing ideal means to mediate catalyst oxidation.



√ single-step access to azetidines from both homo- and allylic amine derivatives
√ mechanistic studies: implication of carbocation intermediate & elucidation of RDS via electrochemical kinetic analysis
√ instillation of pharmaceutical motifs in azetidines
√ other 4-membered heterocycle examples: oxetane, thietane



from Celecoxib

Symposium : **MEDI1-1**

Award Lecture: Excellence in Medicinal Chemistry

Convention Hall 1 THU 15:40

Chair: Sang Min Lim (KIST)

Therapeutic Approaches targeting 3R/4R Tauopathies for the Treatments of AD and PSP

Ae Nim Pae

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

Tauopathies are neurodegenerative disorders characterized by accumulation of tau in neurons or glial cells. Several neuropathologic phenotypes are distinguished based on the distinct anatomic areas and specific isoforms of tau (3R/4R) in pathologic deposits. As tauopathies are strongly linked with neurodegenerative disease, there have been a growing interest in tau-targeted drug discovery. Therefore, we studied and developed novel tau-targeted therapeutic drug candidates for the treatment of AD and PSP by inhibition of tau oligomerization in early stage.Highly potent lead compounds were identified having selective inhibition of 3R/4R tau aggregation by using 3R/4R Tau-BiFC, disease-specific cell-based assay platform and in vivo Tau-BiFC P301L Tg mice model, that improved significantly cognitive and motor dysfunction, and reduced tau pathology with good pharmacological properties.

Symposium : **MEDI1-2**

Award Lecture: Excellence in Medicinal Chemistry

Convention Hall 1 THU 16:25

Chair: Sang Min Lim (KIST)

PHI-501, a novel pan-RAF/DDRs dual kinase inhibitor, overcomes BRAF or MEK inhibitor resistance in melanoma

Ky-Youb Nam

Pharos iBio Co., Ltd., Korea

PHI-501 is a highly effective, and orally accessible dual inhibitor for pan-RAF/DDR that is a collagen-activated receptor tyrosine kinase. Big data and artificial intelligence (AI)-based drug discovery platform and cell-based investigation selected and identified as potentially repurposable PHI-501 against metastatic melanoma. BRAF activated by the common V600E and other mutations, as well as by upstream NRAS mutation are frequent in malignant melanoma, regardless of the therapeutic effect of selective BRAF mutant inhibitors, melanoma patients whose have BRAF non-V600/RAS mutation remain limited response. The major drawback of melanoma treatment is the innate and acquired drug resistance to MAPK inhibitors. In this study, we investigated the inhibitory effects of a novel compound, PHI-501 on resistance to known BRAF and MEK inhibitors in melanoma. In SK-MEL-3, PHI-501 was 47-fold more effective than the class I BRAF inhibitor, dabrafenib (GI50: 0.08 μM vs 3.73 μM). Established dabrafenib- or trametinib-resistant SK-MEL-3 cells were extremely sensitive to PHI-501 (GI50: 0.20 μM and 0.13 μM), whereas their sensitivity to dabrafenib or trametinib was diminished (GI50: NA and 39.61 μM). Comparing the potency of PHI-501 to cobimetinib in acquired resistant SK-MEL-30 cells showed that PHI-501 had 74-fold more inhibitory effect on cell proliferation (GI50: 0.55 μM to 40 μM). PHI-501 inhibited the growth of drug-resistant melanoma cells as effectively as the original drug-naïve cells, and western blot analysis revealed considerable suppression of DDR1/2, ERK, and AKT phosphorylation in MAPK inhibitor-resistant cells. The results of this study suggest that PHI-501, as a single agent, has the potential to overcome the restricted response in the treatment of melanoma.

Symposium : **MEDI1-3**

Award Lecture: Excellence in Medicinal Chemistry

Convention Hall 1 THU 16:50

Chair: Sang Min Lim (KIST)

Discovery of a novel [1,2,4]triazolo[4,3-a]quinoxaline-Based Potent and BD1-Selective BET Bromodomain Inhibitors for the Treatment of Acute Myeloid Leukemia

Kwangho Lee

Korea Research Institute of Chemical Technology, Korea

Bromodomain and extra-terminal (BET) proteins, a class of epigenetic reader domains has emerged as a promising new target class for small molecule drug discovery for the treatment of cancer, inflammatory, and autoimmune diseases. Starting from in silico screening campaign, herein we report the discovery of DW-71177, a novel BET inhibitors based on [1,2,4]triazolo[4,3-a]quinoxaline, which preferentially interacts with BD1 and shows potent antileukemic activity. Isothermal titration calorimetry and molecular dynamic studies revealed strong and selective binding of DW-71177 to the Kac-binding pocket of BD1. DW-71177 suppressed oncogenes as strongly as the pan-BET inhibitor OTX-015, but with a milder effect on housekeeping genes. DW-71177 efficiently blocked cancer-associated transcriptional changes by inhibiting genes highly enriched with BRD4 and histone acetylation marks, suggesting that BD1-selective targeting could be an effective and safe therapeutic strategy against leukemia.

Symposium : **MEDI1-4**

Award Lecture: Excellence in Medicinal Chemistry

Convention Hall 1 THU 17:15

Chair: Sang Min Lim (KIST)

Exploiting interaction between aurora kinase-activator for thrapeutic intervention

Ingyun Lee

ChemicalKinomics center, Korea Institute of Science and Technology, Korea

Aurora kinase A (AURKA) performs critical functions in mitosis. Thus, the activity and subcellular localization of AURKA are tightly regulated and depend on diverse factors including interactions with the multiple binding cofactors. How these different cofactors regulate AURKA to elicit different levels of activity at distinct subcellular locations and times is poorly understood. Using biophysical, structural and cellular methodologies, we have identified a conserved region of CEP192, the major cofactor of AURKA, that mediates the interaction with AURKA. Quantitative binding studies were performed to map the interactions of a conserved helix (Helix-1) within the CEP192. The crystal structure of the Helix-1 bound to AURKA revealed a distinct binding site that is different from other cofactor proteins such as TPX2. Inhibiting the interaction between Helix-1 and AURKA in cells led to the mitotic defects, demonstrating the importance of the interaction. Collectively, we revealed a structural basis for the CEP192-mediated AURKA regulation at the centrosome, that is distinct from TPX2-mediated regulation on the spindle microtubule. By exploiting the protein-protein interaction surface, we aim to develop a novel therapeutic intervention that can selectively disrupt the interaction between AURKA and its activator, to inhibit aberrant mitotic progress.

Symposium : **MEDI2-1**
Recent Trends in Drug Discovery Using DNA Encoded Library Technology
Convention Hall 1 FRI 09:00
Chair: Kyu Myung Lee (KRICT)

Spiro Building Blocks for DNA Encoded Library (DEL) and Medicinal Chemistry

Jung-Nyoung Heo

Therapeutics and Biotechnology Division, Korea Research Institute of Chemical Technology, Korea

This presentation introduces the recent research trends surrounding spiro building blocks in DNA encoded libraries (DEL) and their significance in medicinal chemistry. Spiro building blocks have solidified their position as integral components in contemporary drug research. Recently, the use of DEL technology for drug discovery has emerged as a groundbreaking method that offers the opportunity to derive excellent drug candidates in a cost-effective manner within a significantly shorter timeframe compared to traditional synthesis or screening methods. In particular, spiro compounds play a pivotal role in drug discovery due to their unique three-dimensional configurations and physicochemical properties. The study delves into the use of spiro building blocks in medicinal chemistry and their strategic applications in DNA encoded libraries. Additionally, the synthesis of natural spiro compound, impatien A, will be discussed.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **MEDI2-2**
Recent Trends in Drug Discovery Using DNA Encoded Library Technology
Convention Hall 1 FRI 09:30
Chair: Kyu Myung Lee (KRICT)

Sgd Fqndajd╥Ak̀bjatqm╥Ahdm̀xlď Reaction for DNA-Encoded Library Technology

Gil Tae Hwang

Department of Chemistry, Kyungpook National University, Korea

DNA-encoded library (DEL) technology was initially proposed by Brenner and Lerner in 1992 and subsequently implemented by GlaxoSmithKline in 2009. Since then, DEL technology has facilitated the construction of combinatorial libraries consisting of 10^6 to 10^{12} small-molecule compounds. It has garnered significant attention as a screening approach that can complement or even replace traditional high-throughput screening methods. The fundamental concept underlying this pioneering technology involves encoding each member of a large compound library with a distinct DNA-based barcode. This encoding enables rapid screening of the compounds, thereby expediting the process of drug discovery. The continuous advancement of DNA-compatible reactions is crucial for constructing high-quality DELs that can encompass a broad array of drug-like molecules. Here, we present the synthesis of diverse 5-arylimidazo[1,2-a]pyridin-3-amine derivatives through a combination of the Suzuki-Miyaura reaction followed by the Groebke-Blackburn-Bienaymé reaction.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **MEDI2-3**
Recent Trends in Drug Discovery Using DNA Encoded Library Technology
Convention Hall 1 FRI 10:00
Chair: Kyu Myung Lee (KRICT)

DNA-encoded libraries of peptidomimetics

Min hyeon Shin[*], **Hyun-Suk Lim**[1,*]

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

Peptidomimetics are emerging as a promising class of therapeutic candidates due to their high metabolic stability, good bioavailability and enhanced receptor affinity and selectivity. Therefore, there is considerable interest in the development of libraries of peptidomimetics as a source of ligands for difficult targets, such as protein-protein interaction surfaces. Here, we have designed and synthesized the diverse scaffolds of peptidomimetics libraries encoded with DNA (DNA-encoded libraries of peptidomimetics), and developed novel screening strategy based on in situ click chemistry.In situ click chemistry is a target-guided synthesis approach where the target protein acts as the biological template. Two (or more) ligands involving azide-alkyne moiety could be brought into close proximity by the target protein and covalently assembled through the cycloaddition. As a result, the highly potent bivalent ligand which is thermodynamically stable and has the most optimized orientation could be developed. These features allow in situ click chemistry to be utilized as the attractive screening method. As a screening strategy, we introduced NanoDEL(Nano-based DNA-encoded library) technology which use the nanoparticles as solid supports to secure huge diversity and DNA as encoding materials. Herein, for the first time, we have developed the screening method based on in situ click chemistry using NanoDELs. As a proof-of-concept study, protein tyrosine phosphatase 1B (PTP1B) was used. From the results of screening, hits showed nanomolar level of inhibitory activity. We anticipate that this newly developed method would be innovative screening tool in the discovery of the potent protein ligands.

Symposium : **MEDI2-4**

Recent Trends in Drug Discovery Using DNA Encoded Library Technology

Convention Hall 1 FRI 10:30

Chair: Kyu Myung Lee (KRICT)

Discovery of Kinase inhibitors from a DNA-Encoded small molecule Library

Taedong Han

Department of Discovery Chemistry, DONG-A ST, Korea

There are various approaches to discovering early hit compounds in the development of small molecule drugs. In particular, various methods are used to discover potential hits in the development of kinase inhibitors. Me-too strategies to avoid existing patents, strategies to discover new scaffolds using artificial intelligence, and using internal libraries. In this presentation, we would like to talk about how to use DNA-encoded libraries technology to discovery hit compounds of kinase inhibitor.

Award Lecture in Division : **MAT1-5**

2023 Selection of BKCS-Materials Chemistry

Room 201+202+203 THU 17:00

Chair: Jongnam Park (UNIST)

Exploring the Wonders of Metal Oxides: A New Hydrogen-Bearing Oxide for Hydrogenation Catalysts

Nam Hwi Hur

Department of Chemistry, Sogang University, Korea

Metal oxides are well-established in various applications such as cathodes in lithium-ion batteries, high-temperature superconductors, and colossal magnetoresistance materials. They are also used as oxidation catalysts but have seen limited use in hydrogenation reactions, traditionally dominated by noble metals like platinum, ruthenium, and palladium. Our recent discovery of a highly active hydrogen-bearing ruthenium dioxide (H_xRuO_2) has changed this landscape. H_xRuO_2 serves as a potent catalyst for hydrogenating aromatic compounds, even at mild conditions, offering exceptional selectivity, especially in transforming functionalized nitroarenes into anilines. Through DFT simulations, we attribute this success to efficient proton dynamics, enabling selective hydrogenation at lower temperatures. H_xRuO_2 opens new possibilities for hydrogenation catalysts, operating effectively at low temperatures, and promises sustainable catalytic transformations. Our findings offer a promising avenue for advancing sustainable and energy-efficient catalytic transformations.

Symposium : **MAT1-1**

2023 Selection of BKCS-Materials Chemistry

Room 201+202+203 THU 15:40

Chair: Sungjin Park (Inha University)

Current state of the BKCS and beyond

Sungjin Park

Department of Chemistry, Inha University, Korea

Current state of the BKCS and future strategy will be discussed. Also, "2023 Selection of BKCS-Materials Chemistry" section will be explained.

Symposium : **MAT1-2**

2023 Selection of BKCS-Materials Chemistry

Room 201+202+203 THU 15:45

Chair: Sungjin Park (Inha University)

Perovskite solar cells: Recent Progress and Future

Nam-Gyu Park

School of Chemical Engineering, Sungkyunkwan University, Korea

Since the seminal report on the 9.7% efficient and 500 h-stable solid-state perovskite solar cell (PSC) in 2012 based on methylammonium lead iodide, power conversion efficiency (PCE) was swiftly increased to over 26% due to unique photophysical property of halide perovskite. PSCs are regarded as a game changer in photovoltaics because of low-cost and high efficiency surpassing the conventional high efficiency thin film technologies. High photovoltaic performance was realized by compositional engineering, device architecture and fabrication methodologies for a decade. Toward theoretical efficiency over 30% along with long-term stability, exquisite control of light management and photo-excited charges are highly required, along with thermodynamic phase stability. In this talk, history and progress of PSC are briefly introduced. Toward stable and higher efficiency PSCs, facet engineering of perovskite films is discussed, which is important approach. A specific crystal facet was found to have strong interaction with photon, leading to high photocurrent. Furthermore, a certain facet was found to be quite stable under moisture and PSC based on a perovskite film with abundant moisture-tolerant facet was remarkably stable in humid atmosphere even without encapsulation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **MAT1-3**

2023 Selection of BKCS-Materials Chemistry

Room 201+202+203 THU 16:10

Chair: Sungjin Park (Inha University)

Atomically Dispersed Metal Catalysts: Unusual Catalytic Selectivity and Active Site Identification

Sang Hoon Joo

Department of Chemistry, Seoul National University, Korea

Atomically dispersed metal catalysts have emerged as a new frontier in heterogeneous catalysis. In addition to the widely perceived advantages of maximized metal utilization and substantially reduced metal content, they have shown different catalytic selectivity compared to the traditional nanoparticle (NP)-based catalysts. We have explored atomically dispersed metal catalysts for electrocatalytic reactions, where the control of selectivity is critical. As a notable exemplar, we present atomically dispersed Pt sites on carbon nanotubes (Pt_1/CNT) as a highly selective electrocatalyst for the chlorine evolution reaction (CER), which is a key anodic reaction in the chlor-alkali electrolyzer. The Pt_1//CNT catalysts with $Pt–N_x$ active sites showed higher CER activity and selectivity than the commercial precious metal-based oxide catalyst (DSA) and Pt NPs on CNT. The Pt_1/CNT preserved ~100% selectivity even in low Cl^- concentration and neutral pH conditions, where the CER is thermodynamically more unfavorable than the OER. Furthermore, Pt_1/CNT exhibited unusual potential-dependent CER kinetics and mechanism, which are clearly distinguishable from those of DSA. We also show that $Pt–N_x$ active sites are composed of multiple sites, among which a genuine active site is identified.

Symposium : **MAT1-4**

2023 Selection of BKCS-Materials Chemistry

Room 201+202+203 THU 16:35

Chair: Sungjin Park (Inha University)

Local Structure Control of Chalcogel for Environmental and Energy Applications

Myung-Gil Kim

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

Chalcogenide aerogels (chalcogels) are typically synthesized with thiolysis, aggregration of nanoparticles, and metathesis of chalcometallate. Especially, the metathesis of chalcometallate enabled generalized synthesis of chalcogel with flexible choice of central metal cations and chalcometallate. Although recent developments of chalcogel achieved high surface area and unconventional surface functionality with chalcogenide, chalcogels are amorphous structures with lack of localized structural control, which hinder further tuning of pore structure, crystallinity and surface functionality. We have investigated local structure of thiostannate and thiomolybdate chalcogels. The precise local structure control of thiomolybdate chalcogel enabled high performance electrocatalyst for hydrogen evolution reaction. Furthermore, the coordination transformation of thiostannate enabled new synthetic route and local structure control of chalcogel. For high performance aqueous radionuclide-adsorption, the well-defined crystalline Na-Mn-Sn-S chalcogel enabled efficient Cs^+ and Sr^{2+} ion exchange reactions.

Award Lecture in Division : **MAT2-4**
Recent Trends in Materials Chemistry for Next-generation Battery
Room 201+202+203 FRI 10:25
Chair: Jongsoon Kim (Sungkyunkwan University)

When Biology Meets Materials Chemistry: the Case of DNA and Inorganic/Organic Nanomaterials

Jae-Seung Lee

Department of Materials Science and Engineering, Korea University, Korea

The integration of biology and materials chemistry has opened up new horizons in science. DNA, for instance, has acquired new functionalities, ranging from genetic information transfer to the assembly of building blocks and target recognition in the field of nanotechnology. For these objectives, the application of biochemical conjugation principles to functionalize nanoscale inorganic and organic materials using DNA is highly valued. In this presentation, I will showcase several successful projects our group has developed over the past decade. These projects focus on synthesizing nanomaterials using noble metals, metal halides, and DNA, exploring their chemical and physical properties, as well as their diagnostic and therapeutic applications. In particular, it is noteworthy that the integration of fundamental disciplines in materials chemistry and biology provides materials chemists with ample opportunity to make significant contributions towards addressing pivotal questions in nanotechnology. Our group has examined various conceptual examples that effectively illustrate this notion, a selection of which will be outlined in this presentation.

Symposium : **MAT2-1**

Recent Trends in Materials Chemistry for Next-generation Battery

Room 201+202+203 FRI 09:00

Chair: Jongsoon Kim (Sungkyunkwan University)

Next-Generation Sulfur Cathode: Electrocatalyst to Accelerate Sulfur Conversion Reaction

Jinwoo Lee

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

Although lithium-sulfur (Li-S) batteries have been expected as a promising high-energy-density battery system, entangled problems in each cell component hamper their practical use. Especially in cathode, low electronic/ionic conductivity of sulfur based active material, continuous dissolution of polysulfide, and sluggish redox kinetics cause the poor cycle stability and energy density. For the energy density of 500~600 W h kg-1, achievement of high areal sulfur loading and low electrolyte to sulfur (E/S) ratio is needed, but conventional carbon/sulfur composite-type cathodes have limitations to satisfy this requirement. In this seminar, next-generation sulfur cathode with the electrocatalyst accelerating the sulfur conversion reaction is introduced as a powerful platform to simultaneously improve the cycle stability, reversible capacity, and rate capability. This seminar aims to present comprehensive overview of previously conducted studies and future research direction to design the efficient electrocatalyst for sulfur cathode. In particular, strategies to search for new electrocatalyst, to improve the catalytic activity and stability of catalyst, and to fundamentally understand the electrocatalytic trends in sulfur cathode will be covered. We believe development of optimized catalytic materials in cathode with the deep fundamental understanding on electrocatalysis enables realization of high areal sulfur loading and low E/S ratio for high energy density of Li-S batteries.

Symposium : **MAT2-2**

Recent Trends in Materials Chemistry for Next-generation Battery

Room 201+202+203 FRI 09:25

Chair: Jongsoon Kim (Sungkyunkwan University)

Enhancing Surface Functionality of Ni-Rich Layered Oxide Cathode for Lithium-Ion Batteries

Junyoung Mun

School of Advanced Materials Science & Engineering, SKKU Institute of Energy Science & Technology (SIEST), Sungkyunkwan University, Korea

IntroductionThe global warming issue is no longer just a conceptual threat as ambient temperatures have rapidly increased in recent years. The main sources of CO2 generation are power plants and vehicles. Highly efficient energy systems, such as electric vehicles and energy storage systems, are being pursued to mitigate this critical issue. One of the main challenges of high-capacity cathode materials (Ni-rich cathode materials) is comprehensively discussed, including material synthesis, side reactions with electrolytes, and changes in crystal structure. To solve this problem, a problem-solving study through self-assembled monolayer functional surface coating is introduced. This gas-phase coating has excellent processability, uniform surface control, and easy surface functionality control according to the introduction of various molecular structures. Furthermore, material crystal/surface structural change is suppressed by low-temperature treatment, energy density is maintained by forming a thin structure in Å units, and output characteristics are maintained.AcknowledgeThis work was supported by the Technology Innovation Program (20010900) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea)

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **MAT2-3**

Recent Trends in Materials Chemistry for Next-generation Battery

Room 201+202+203 FRI 09:50

Chair: Jongsoon Kim (Sungkyunkwan University)

Design and Process Development of Thick Cathodes for Next-Generation Lithium-Ion Batteries

Jung-Keun Yoo[*], **Jihee Yoon**[1]

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

[1]*Korea Institute of Materials Science, Korea*

Recently, in order to enhance the energy density of lithium secondary batteries, research has been conducted not only on the development of high-capacity materials but also on the design of thick cathodes (~ 8 mAh/cm2) . When applying high-capacity active materials within the cathode at a high ratio and increasing the thickness of the cathode, it is very effective for designing high-energy density batteries, and it has the advantage of reducing the number of electrode stacks, thereby lowering the production cost of the battery. However, for stable operation of high-energy density thick cathodes, movement of lithium ions and electrons in the direction of cathode thickness is essential. To achieve this, it is necessary to develop new forms of conductive materials and binders, as well as processes that induce uniform distribution of the cathode materials. This presentation includes the development of high surface area and high conductivity carbon nanotube (CNT) conductive materials, as well as novel thermoset binders with high adhesion and ion conductivity for implementing high-energy density thick cathodes. Additionally, in order to achieve uniform material distribution within the thick cathodes, a high-concentration (cathode slurry solid content ~ 80 wt%) slurry manufacturing method that minimizes solvent evaporation and solvent-free dry processes are introduced to present the electrochemical characteristics of the fabricated thick cathodes.

Symposium : **MAT3-1**
From Synthesis to Application of Nanomaterials with Quantum Properties
Room 201+202+203 FRI 14:30
Chair: In Young Kim (Ewha Womans University)

Research Trends of Spintronics Materials and Devices

Taegweon Lee

Department of Chemistry, Ajou University, Korea

Semiconductor-based electronic devices have led the information age through rapid technological progress. However, since it is facing technical limitations in fundamental physical phenomena and nano-processes, it is necessary to emerge a new next-generation electronic device that can overcome that issues. Molecular electronics, nanoelectronics, spintronics, and quantum information technology were proposed as new methodologies. Among them, spintronics is a compound word of 'spin' and 'electronics', which is a technology that utilizes the spin of electrons. This technology has various potential advantages such as non-volatility, high integration, low energy consumption, and improved data processing speed because it can control and use spin-up and spin-down as well as electron charge. In this presentation, we will summarize the characteristics and application status of each type of spintronic material, which has not yet been actively approached from the material side, despite its advantages. In addition, based on this, we will review the requirements necessary to achieve technological progress. Depending on their electronic and magnetic properties, spintronic materials can be broadly classified into magnetic metals, topological insulators(TIs), and magnetic semiconductors. According to this category, we would like to introduce R&D trends for each organic and inorganic materials.

Symposium : **MAT3-2**

From Synthesis to Application of Nanomaterials with Quantum Properties

Room 201+202+203 FRI 14:55

Chair: In Young Kim (Ewha Womans University)

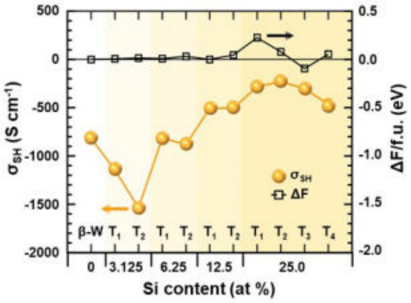
Spin-orbit torque switching materials for nonvolatile embedded memory applications

Young Keun Kim

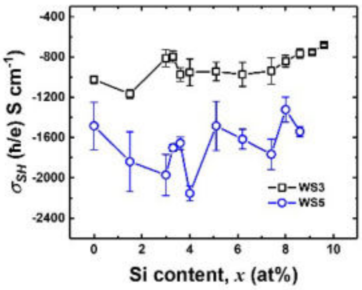
Department of Materials Science and Engineering, Korea University, Korea

Spin-orbit torque (SOT) based magnetization switching is of current technological interest to demonstrate its utilization in nonvolatile embedded memory such as magnetic random access memory (MRAM), logic devices, and true random number generators. These devices require a few nanometer-thick materials with perpendicular magnetic anisotropy (PMA) for high bit density, significant SOT efficiency to warrant low power consumption, and external field-free magnetization switching. Above all, materials must be semiconductor fabrication-friendly. However, only a few materials and their heterostructures previously explored fulfill the requirements. Lately, we have investigated the β-phase W thin film and its alloys, such as W-V, W-N, and W-Si, as the spin current-generating layer. We use equilibrium phase diagrams and first-principles energy band calculations to narrow down the compositional ranges where we can get high spin Hall conductivity values. Then, we deposit nonmagnet/ferromagnet heterostructures and pattern them into Hall bar devices. For example, we confirm that the heterostructure consisting of W-Si (4 at%)/CoFeB exhibits PMA, a high damping-like SOT efficiency (~0.58), and low longitudinal resistivity (~135 μΩ cm). Furthermore, we estimate ten times smaller write power consumption than the heterostructure based on the pristine β-W.

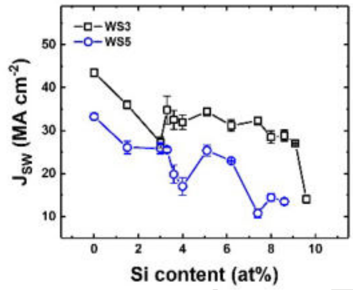
Fig. 1. SOT-driven magnetization reversal process for potential applications in MRAM devices. The designed material retains a β-W phase and exhibits perpendicular magnetic anisotropy, high SOT efficiency, low resistivity, and field-free switching.



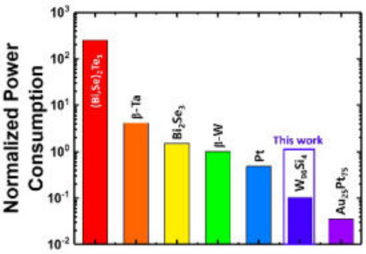
σ_{SH} (S cm^{-1})
ΔF/f.u. (eV)
500
0
-500
-1000
-1500
-2000
0.5
0.0
-0.5
-1.0
-1.5
-2.0
σ_{SH}
ΔF
β-W
T_1
T_2
T_3
T_4
0
3.125
6.25
12.5
25.0
Si content (at %)



σ_{SH} (ħ/e) S cm^{-1})
-400
-800
-1200
-1600
-2000
-2400
WS3
WS5
0
2
4
6
8
10
Si content, x (at%)



J_{SW} (MA cm^{-2})
50
40
30
20
10
WS3
WS5
0
2
4
6
8
10
Si content (at%)



Normalized Power Consumption
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
$(Bi_2Se)_2Te_3$
β-Ta
Bi_2Se_3
β-W
Pt
This work
$W_{96}Si_4$
$Au_{25}Pt_{75}$

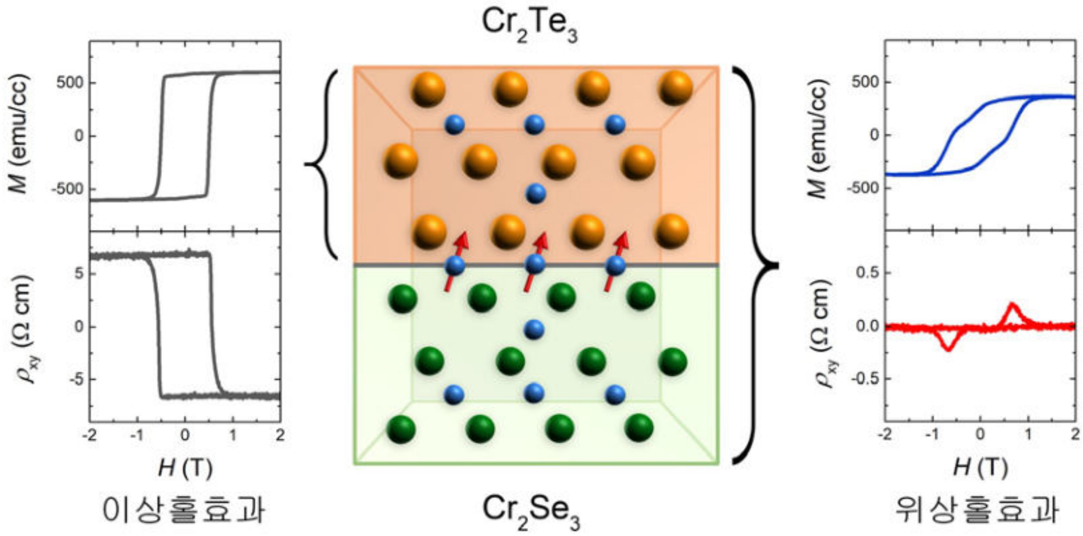
Symposium : **MAT3-3**
From Synthesis to Application of Nanomaterials with Quantum Properties
Room 201+202+203 FRI 15:20
Chair: In Young Kim (Ewha Womans University)

Molecular beam epitaxy and exotic Hall effects in topological quantum systems

Seung-hyun Chun

Department of Physics and Astronomy, Sejong University, Korea

The Hall effect refers to the voltage transverse to the current direction in a conductor under a perpendicular magnetic field. As the Hall effect is sensitive to the current density and/or the magnetic field, it is widely used in power generation systems, mobile phones, robot controls, cars, or the global positioning system. It is also a valuable tool for identifying quantum systems. The topological matters, such as the two-dimensional electron gas, graphene, topological insulators, or skyrmions exhibit exotic Hall effects: from quantum Hall effects to topological Hall effects. We will present the history of various Hall effects along with the introduction of Molecular Beam Epitaxy (MBE), the indispensable film growth system for topological quantum materials.



Cr_2Te_3
Cr_2Se_3
M (emu/cc)
ρ_{xy} (Ω cm)
H (T)
500
0
-500
5
-5
0.5
0.0
-0.5
-2
-1
0
1
2
이상홀효과
위상홀효과

Symposium : **MAT3-4**

From Synthesis to Application of Nanomaterials with Quantum Properties

Room 201+202+203 FRI 15:45

Chair: In Young Kim (Ewha Womans University)

Understanding the Quantum Revolution: A Simplified Overview for Materials Chemists

Youngwook Kim

Daegu Gyeongbuk Institute of Science & Technology, Korea

In this presentation, we will explore the exciting world of quantum computing, a technology that's set to revolutionize the way we process information. We'll highlight the latest advancements in different designs of quantum computers - from the transmon qubit to the spin and topological qubits. Additionally, we'll touch on the unique materials and structures, like the van der Waals heterostructure, that make these quantum systems possible.

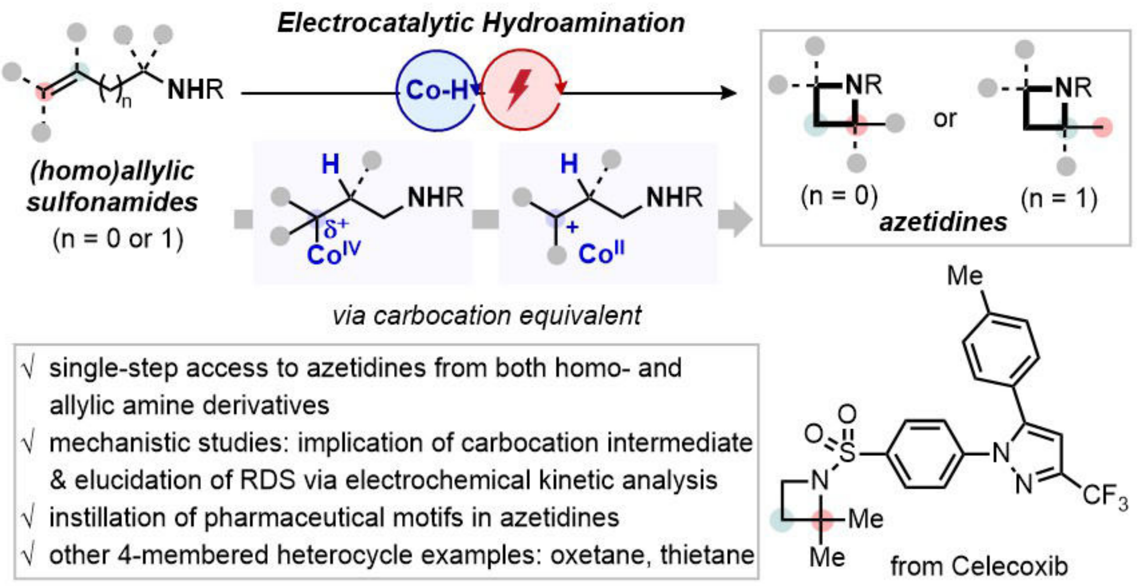
Symposium : **ELEC1-1**
Electrochemical Organic Synthesis: Electrochemistry and Organic Chemistry
Room 206+207 THU 15:40
Chair: Chang Hyuck Choi (POSTECH)

Cobalt-Electrocatalyzed Radical-Polar Crossover Hydrofunctionalization of Alkenes

Hyunwoo Kim

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

Due to the unique reactivity of open-shell intermediates, the development of catalytic transformations driven by single-electron transfer (SET) has been an area of intense research in organic chemistry. In particular, the employment of unconventional means of activation, including photoredox catalysis and electrocatalysis, has provided unique entry to single-electron reactivities and led to new solutions to challenging synthetic problems that are not readily addressed using existing tools. We disclose a general electrocatalytic hydrofunctionalization by utilizing a wide range of alkenes. The integration of the two involves an electrochemically instigated cobalt-hydride-catalyzed radical-polar crossover of alkenes that enable the generation of key cationic intermediates, which could readily be entrapped by challenging nucleophiles. We highlight the importance of precise control of the reaction potential by electrochemistry in conjunction with the decisive role of 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) as the co-solvent to obtain optimal and exclusive chemoselectivity. In addition, we develope an electrocatalytic method for intramolecular hydroamination of allylic sulfonamides to access azetidines. The merger of cobalt catalysis and electricity enables regioselective generation of key carbocationic intermediates, which could directly undergo intramolecular C-N bond formation. The mechanistic investigations including electrochemical kinetic analysis suggest that the catalyst regeneration by nucleophilic cyclization is involved in the rate-determining step (RDS) of our electrochemical protocol and highlight the ability of electrochemistry in providing ideal means to mediate catalyst oxidation.



√ single-step access to azetidines from both homo- and allylic amine derivatives
√ mechanistic studies: implication of carbocation intermediate & elucidation of RDS via electrochemical kinetic analysis
√ instillation of pharmaceutical motifs in azetidines
√ other 4-membered heterocycle examples: oxetane, thietane

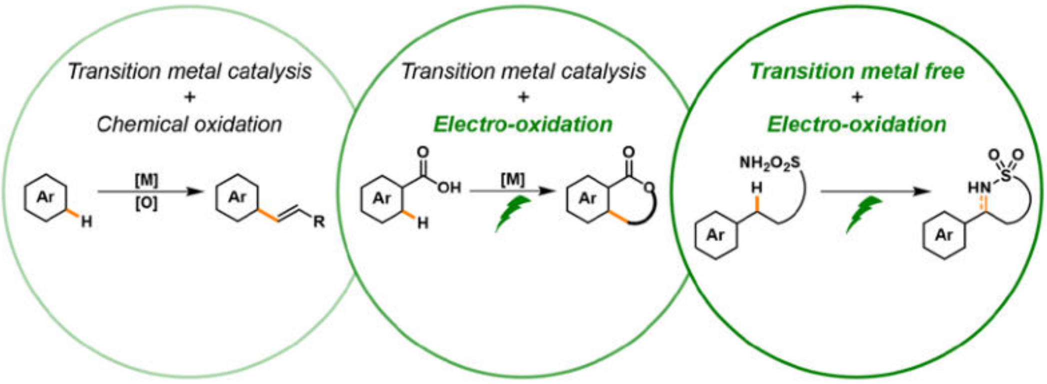
Symposium : **ELEC1-2**
Electrochemical Organic Synthesis: Electrochemistry and Organic Chemistry
Room 206+207 THU 16:05
Chair: Chang Hyuck Choi (POSTECH)

A Way Towards Sustainable C–H Bond Functionalization

Isaac Choi

Department of Chemistry, Chungbuk Natioanl University, Korea

C–H bond manipulation provides chemists with efficient and step-economical strategies in organic syntheses. However, classical oxidative/reductive transformations still require suprastoichiometric amounts of terminal oxidants or reductants, which generate a large quantity of chemical wastes and thereby prevent sustainable chemistry. In this talk, I present my recent research efforts toward the achievement of sustainable organic syntheses, spanning from transition metal-catalyzed oxidative C–H activation to metallaelectrooxidative C–H activation and electro-tunable divergent C–H functionalization.



132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **ELEC1-3**

Electrochemical Organic Synthesis: Electrochemistry and Organic Chemistry

Room 206+207 THU 16:30

Chair: Chang Hyuck Choi (POSTECH)

Progress in Electrochemical Synthesis of (Hetero)aromatic Compounds: Efficient Generation of 1H-Indazole N-oxides and Selective Assembly of 1,3,5- and 1,2,4-Trisubstituted Benzenes

Jin Kyoon Park

Department of Chemistry, Pusan National University, Korea

Modern organic chemistry focuses on developing sustainable chemical reactions that reduce or eliminate the production of hazardous pollutants. Transition metal catalysts are utilized in traditional strategies to minimize by-products. To achieve a sustainable approach, organic chemistry has integrated with emerging technologies like electrochemistry, enabling previously challenging reactivity and selectivity. Electrochemical synthesis, which leverages the advantages of pure electrons replacing chemical redox reagents, has gained significant attention as an ideal tool for organic transformations.

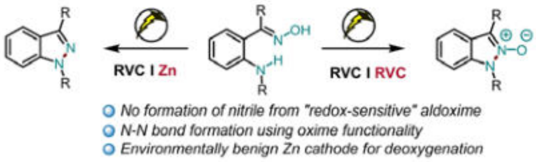
The first part of our study describes the selective electrochemical synthesis of 1H-indazoles and their N-oxides, followed by the subsequent CH functionalization of the 1H-indazole N-oxides.[1] The electrochemical outcomes are influenced by the cathode material used. Utilizing a reticulated vitreous carbon cathode enables the selective synthesis of a wide range of 1H-indazole N-oxides. Conversely, employing a Zn cathode results in the deoxygenation of electrosynthesis products, leading to the formation of N-heteroaromatics through cathodic cleavage of the N-O bond via paired electrolysis.

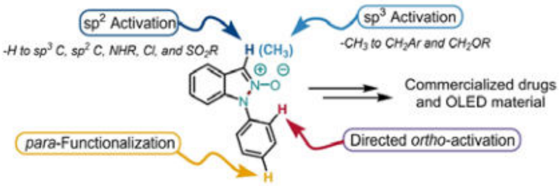
The second part presents a unified electrochemical synthetic strategy for paired electrochemical [2 + 2 + 2] cyclotrimerizations of terminal alkynes.[2] This approach allows selective access to both 1,3,5- and 1,2,4-regioisomeric trisubstituted benzene derivatives.

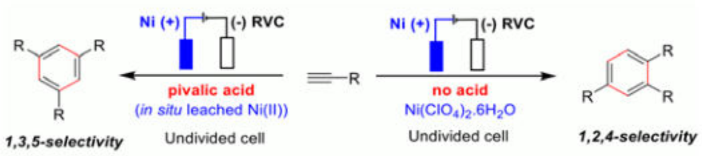
References

[1] Arepally, S; Kim, T.; Kim, G.; Yang, H.; Park, J. K.* Angew. Chem. Int. Ed. 2023. 62, e202303460 (Hot Paper).

[2] Arepally, S.; Nandhakumar, P.; González-Montiel, G. A.; Dzhaparova, A.; Kim. G.; Ma, A.; Nam, K. M.; Yang, H.*; Cheong, P. H-Y*; Park, J. K* ACS Catalysis, 2022, 12, 6874 (Supplementary Journal Cover).







132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ELEC1-4**
Electrochemical Organic Synthesis: Electrochemistry and Organic Chemistry
Room 206+207 THU 16:55
Chair: Chang Hyuck Choi (POSTECH)

Sustainable Electrified Imine Chemistry

<u>Kyoungsuk Jin</u>

Chemistry Department, Korea University, Korea

Imines, characterized by carbon-nitrogen double bonds, are pivotal in diverse chemical syntheses including the production of dyes, pharmaceuticals, and natural products. Among these, ketone-derived imines (ketimines) hold substantial significance due to their capacity to incorporate intricate moieties. Nevertheless, the limited reactivity of ketones poses a significant hurdle in ketimine formation, prompting exploration into the methylation of aldehyde-based imines (aldimines) as an alternative strategy. Moreover, the introduction of methyl groups into molecules can induce alterations in their physical and chemical attributes, physiological activity, and target selectivity. In the realm of medicinal chemistry, this phenomenon coined the "magic methyl" effect, has been extensively investigated to enhance drug efficacy. While some methodologies for aldimine methylation have been demonstrated using photochemical reactions or transition metal catalysts, these approaches necessitate multiple additives and intricate, multi-step procedures. This study introduces a direct electrochemical methylation strategy employing dimethyl sulfoxide as both solvent and methyl source. We systematically optimized catalytic performance by evaluating diverse electrode materials, solvent-electrolyte combinations, and supplementary additives. We believe that our approach delineates an environmentally conscious, streamlined pathway for one-pot ketimine synthesis. Furthermore, we propose that this method opens doors to intricate organic electro-synthetic reactions, as the sp2 carbon framework remains unaltered.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ELEC1-5**

Electrochemical Organic Synthesis: Electrochemistry and Organic Chemistry

Room 206+207 THU 17:20

Chair: Chang Hyuck Choi (POSTECH)

Interfacing Electrochemistry with Organic Chemistry

Taek dong Chung

Department of Chemistry, Seoul National University, Korea

Electro-organic chemistry, which involves redox reactions at the electrode–electrolyte interface, has been gaining renewed attention. From an organic chemistry point of view, electrodes and electrons are treated as ‘traceless redox agents’. However, the phenomena occurring in the vicinity of the electrode are strongly dependent on the type of electrode materials and yet less explored. The environment of the electrical double layer (EDL) can also profoundly impact the stability of intermediates and thereby influencing the reaction outcome.In the first half of this talk, we will introduce our recent research advances regarding the influence of electrode material and EDL environment on the reaction mechanism. Using a thin layer cell, the importance of selecting an appropriate potential was revisited due to the capability of multiple electrons being transferred, resulting in the formation of different reaction intermediates. A semiconductor photoanode could directly oxidize aromatic substrates at a controllable rate by regulating illumination intensity, thereby making selective radical–radical coupling reactions possible. Reactive hydrogen species were electrochemically generated at a silicon oxide layer, which enabled the activation of anthracene derivatives.In the second part, we will present our perspective on the future direction of electro-organic chemistry. Spectroscopic techniques can provide insights into the interaction between the electrode surface and reaction intermediates. Electrochemical methods other than cyclic voltammetry can also provide powerful evidence for mechanistic investigations. Overall, we believe that a novel paradigm of electro-organic chemistry will be established through our understanding of the phenomena at the heterogeneous interface.

Award Lecture in Division : **ELEC2-5**
Electrocatalytic Reactions for Carbon Neutrality
Room 206+207 FRI 10:40
Chair: Yun Jeong Hwang (Seoul National University)

Voltammetric Nanobiosensing Approaches for Biomedical and Environmental Applications

Hye Jin Lee

Department of Chemistry, Kyungpook National University, Korea

In this talk, I will highlight our latest efforts made on the development of electrochemical biosensing approaches utilizing biofunctionalized nanoparticles for biomedical and environmental applications. A concerted methodology was established via combining various metallic and non-metallic or hybrid nanoparticles decorated with bio-receptor molecules specific to a target analyte and a novel sandwich assay involving a pair of bio-receptors alongside surface enzyme process. As an example, voltammetric analyses of disease related biomarkers and environmentally toxic agents using enzymatically amplified or surface sandwich assay platforms integrating different sets of antibody-DNA aptamer receptor pairs alongside biofunctionalized nanomaterials will be presented. Finally, future aspects and challenging issues of our biosensing technologies will be discussed.

Symposium : **ELEC2-1**

Electrocatalytic Reactions for Carbon Neutrality

Room 206+207 FRI 09:00

Chair: Yun Jeong Hwang (Seoul National University)

Non-Precious Electrocatalysts-Based Anion Exchange Membrane Water Electrolysis with Superior Performance

Sung Mook Choi

Surface & Nano Materials Division, Korea Institute of Materials Science, Korea

The development of highly active electrocatalysts, electrodes, and membrane electrode assembly (MEA) is crucial for the practical implementation of a water electrolysis system, which is essential for the production of pure hydrogen and the commercialization of water electrolyzers. In this study, Co-based non-precious group metal (PGM) oxide electrocatalysts were synthesized for the oxygen evolution reaction (OER) using co-precipitation, electro-deposition method, and so on. These catalysts were subsequently applied as anode electrodes in an anion exchange membrane water electrolyzer (AEMWE). We easily and creatively developed nano-sized Co-based oxide catalysts with abundant oxygen vacancies, large electrochemical surface area, morphology control, and electronic modification by using several synthesis methods. As a result, the catalyst demonstrated superior catalytic activity and long-term stability in half-cell tests. Recent reports have mainly focused on the catalytic activity of electrocatalysts in half-cell tests. However, it is crucial for electrocatalysts to exhibit excellent performance in full-water electrolysis cells to achieve commercial viability. In this study, we not only compared the catalytic activity of the synthesized catalyst but also applied it directly to a full AEMWE cell to evaluate its practical hydrogen production performance. The AEMWE cell's performance surpassed that of any previously reported AEMWE cells, even when compared to those using IrO2 as an anode catalyst.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **ELEC2-2**
Electrocatalytic Reactions for Carbon Neutrality
Room 206+207 FRI 09:25
Chair: Yun Jeong Hwang (Seoul National University)

Catalyst developments for the electrochemical conversion of hydroxymethylfurfural (HMF) to furandicarboxylic acid (FDCA)

Dong Ki Lee

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

The electrochemical conversion of biomass-derived 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA) has been considered the most promising oxidation reaction that can be paired with CO2 conversion and H2 evolution reaction, among the various electrochemical organic oxidation reactions. This is because the molecular structure of FDCA is similar to terephthalic acid, thus the FDCA can be used as an alternative building block replacing terephthalic acid in producing various chemicals and plastics. Previous studies reported excellent performance over 90% of FDCA yield and Faraday efficiency (FE) in 1.0 M KOH or NaOH conditions (≈ pH 14). However, the pH 14 electrolyte condition is hard to apply for practical HMF to FDCA conversion process because the base-induced polymerization of HMF is greatly accelerated under high concentrations of OH-, resulting in rapid degradation of HMF to useless humins. In this respect, developing electrocatalysts with excellent reactivity under pH 13 conditions is still in demand. In this talk, I will present the primary factor causing HMF degradation and catalyst designs for preventing HMF degradation under alkaline conditions.

Symposium : **ELEC2-3**

Electrocatalytic Reactions for Carbon Neutrality

Room 206+207 FRI 09:50

Chair: Yun Jeong Hwang (Seoul National University)

Liquid-diffusion electrode with core-shell structured mixed metal oxide catalyst for near-zero polarization in chlor-alkali electrolysis

Chan Woo Lee

Department of Applied Chemistry, Kookmin University, Korea

Chlor-alkali electrolysis is a key industrial process for the production of chlorine gas, caustic soda, and hydrogen fuels. Here, we demonstrate that a Ti foam electrode, which has a diffusion layer of liquid reactant, deposited with a thin layer of core/shell-structured mixed metal oxide nanoparticles enables almost zero polarization in the range of hundreds of mA/cm2 towards the chlorine evolution reaction (CER), using noble-metals 20 times lower than commercial electrode. The fast charge-transfer kinetics induce near-zero overpotential at low current densities, while the high mass transport rates aided by porous channels lead to unprecedentedly high CER performance. Under practical chlor-alkali process conditions, the mixed metal oxide electrode exhibited remarkable performance as a bifunctional electrode for CER and hydrogen evolution reaction (HER) with overpotential of 11 mV for HER.

Symposium : **ELEC2-4**

Electrocatalytic Reactions for Carbon Neutrality

Room 206+207 FRI 10:15

Chair: Yun Jeong Hwang (Seoul National University)

In-situ Tracking Active Phases in The Oxygen Evolution Reaction on Transition Metal (Oxy)hydroxides

Seunghwa Lee

Department of Chemical Engineering, Changwon National University, Korea

The oxygen evolution reaction (OER) is considered as the bottleneck reaction for electrochemical water splitting, which can be potentially used to produce the hydrogen fuel in a sustainable manner with renewable energies from the sun and wind. Despite great efforts devoted to the development of catalysts composed of only Earth-abundant elements, the understanding of these catalysts remains unclear. Take cobalt iron oxyhydroxides (CoFeOxHy) as an example. This catalyst has been widely known as one of the most promising active materials in alkaline medium, but there was no consensus on whether Co or Fe sites were intrinsically responsible for the OER catalysis. In this work, in-situ ultraviolet-visible (UV-Vis) spectroscopy and Raman spectroscopy were employed to investigate the nature of CoFeOxHy catalysts during OER. Various Co and Fe species were identified to be formed with respect to the applied potential. Our analysis reveals that surface Fe^{4+} species rather than bulk Co^{4+} species are likely the active sites for OER on CoFeOxHy. This work enhances the understanding of the nature of active phases for a benchmark OER catalyst. The methods presented in this work might be applied to study the active phases of other OER catalysts.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ELEC3-1**

Emerging Trends in Fundamental Electrochemistry

Room 206+207 FRI 14:30

Chair: Jun Hui Park (Chungbuk National University)

Polymer Characterization Using Electrochemistry: Observing Molecular Weight and Phase Transitions

Byung-Kwon Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The cloud point temperature (Tcp) is a key thermal parameter utilized to characterize the phase transition behavior in thermoresponsive polymers. In the context of this research, electrochemical techniques were employed to determine an electrochemical cloud point temperature (Tecp), offering enhanced accuracy in identifying the phase transition temperature compared to the traditional Tcp. This was achieved through the application of thermoamperometry using an ultramicroelectrode, with poly(arylene ether sulfone) (PES10) serving as the representative polymer. The Tecp of PES10 was derived from the resulting real-time current-temperature (i-T) profile. Interestingly, the i-T profile exhibited a remarkable decrease in current as the temperature of the PES10 solution increased. In contrast, the solution lacking PES10 showed a linear increase in current with rising temperature. A comprehensive analysis of this phenomenon was conducted, taking into account various factors associated with PES10 during the phase transition, including dynamic viscosity, solution temperature, and electrode impedance. It was established that the primary reason for the observed decrease in current within the i-T profiles was primarily attributed to the contraction of the effective electrode surface area. A comparative evaluation between Tecp and Tcp demonstrated their similar dependence on the concentrations of the thermoresponsive polymer and the supporting electrolyte. These findings emphasize the potential of manipulating polymer and electrolyte concentrations in organic solutions to effectively harness Tecp as an innovative analytical tool. This methodology holds promise for applications in electric circuit-based energy storage devices such as lithium-ion batteries and supercapacitors.

Symposium : **ELEC3-2**
Emerging Trends in Fundamental Electrochemistry
Room 206+207 FRI 14:55
Chair: Jun Hui Park (Chungbuk National University)

New Electron Mediators for Electrochemical Point-of-Care Testing

Haesik Yang

Department of Chemistry, Pusan National University, Korea

The commonly required properties of diffusive electron mediators for point-of-care testing are rapid dissolubility, high solubility, high stability, and moderate formal potential in aqueous solutions. Various electron mediators have been developed; however, satisfying all these requirements remains a challenge. A strategic design toward quinones incorporating sulfonated thioether and nitrogen-containing heteroarene moieties as solubilizing, stabilizing, and formal potential-modulating groups will be presented. Moreover, a new ferrocene compound containing two electron-withdrawing acyl substituents and eight electron-donating methyl substituents will be presented.

Symposium : **ELEC3-3**

Emerging Trends in Fundamental Electrochemistry

Room 206+207 FRI 15:20

Chair: Jun Hui Park (Chungbuk National University)

Electrochemical Application of Liquid Organic Hydrogen Carriers

Sang-Il Choi

Department of Chemistry, Kyungpook National University, Korea

Since hydrogen is difficult to store and transport in gaseous form, thermochemical liquid organic hydrogen carriers (LOHCs) have been developed as one of the alternative H_2 storage technologies. However, the high temperature and pressure requirements of thermochemical LOHC systems result in significant energy waste and impracticality. This presentation proposes an electrochemical (EC)-LOHCs system to store and utilize H_2 more efficiently and safely at lower temperatures and pressures. To enable this system, several EC-LOHC candidates, including isopropanol, phenolic compounds, and organic acids, will be discussed. The latest research trends and design concepts of related homo/hetero-based electrocatalysts will also be presented. Finally, efficient fuel cell-based systems implementing EC-LOHCs will be shared. This presentation invites open discussion with attendees to share ideas for developing related technologies.


Organic
2
OH
OH
OH
HO
OH
OH
OH
HO
OH

Symposium : **ELEC3-4**

Emerging Trends in Fundamental Electrochemistry

Room 206+207 FRI 15:45

Chair: Jun Hui Park (Chungbuk National University)

Micro/Nanoscale Electrochemistry for Enhanced Chemical Detections and Molecular Dynamic Studies

Paul Bohn*, Henry White[1,*], Seol Baek[2]

Department of Chemistry & Biochemistry, University of Notre Dame, United States

[1]*Department of Chemistry, University of Utah, United States*

[2]*Chemistry, Sookmyung Women's University, Korea*

Nanopore electrode arrays (NEAs), are useful architectures to investigate a number of interesting nanoelectrochemical characteristics in confined volumes, *typ.* 10^{-18} L. Also, this small confined volume makes it possible to explore dynamics of chemical reactions involving a single or a few molecules. The first topic focuses on the demonstration of biomimetic ion gating in block copolymer (BCP)-coated NEAs in response to external stimuli, such as pH and ionic charge state. The BCP membrane serves as a pH-gate, controlling ion transfer into the nanopores, owing to pH-dependent structural transitions. Redox species are selectively transported through the BCP into NEAs where they can then be sensitively detected by electrochemical signal amplification by redox cycling. Extending this concept, potential-induced wetting and dewetting behavior is characterized in BCP membranes on NEAs. Interestingly, mass transport across the hydrophobic BCP nanochannels is switched on by sufficiently-negative potentials applied across the BCP membrane, resulting in the electrolyte solution being introduced and isolated in the nanopores. Moreover, NEAs are used in a bifunctional zero mode waveguide (ZMW) that combines electrochemistry with spectroscopy for single enzyme molecule studies. The potential-dependent fluorescence dynamics of enzyme molecules are investigated in an electrochemical ZMW, where a single Au ring nanoelectrode simultaneously serves to control potential and to confine electromagnetic radiation in a zeptoliter-scale observation volume. The last topic addresses microscale ion-selective electrodes with scanning electrochemical microscopy to investigate autocatalytic reaction-associated mass transport and local activities of surface-bound enzyme.

Symposium : **EDU1-1**

Current Issues and Research in Chemistry Education

Room 304 FRI 09:00

Chair: Wonho Choi (Sunchon National University)

The Roles of Schools and University with Respect of Mathematical & Computational Thinking Focused in the 2022 National Curriculum Revision

Dae Hong Jeong

Department of Chemical Education, Seoul National University, Korea

National curriculum was officially revised and announced in 2022, which is documented as “The 2022 National Curriculum Revision”. Compared with the previous curriculum of The 2015 National Curriculum Revision”, this revision highlights literacies such as “AI-digital literacy” and “Ecological Transformation Education”. Among them the former literacy is more focused in natural science education while the latter is in social science education. In fact, digital literacy was also emphasized in the previous 2015 curriculum revision. In the current curriculum, digital literacy is even more strongly emphasized from elementary level to high school level such that specific requirements for digital literacy is described in each achievement standard.

There are several domains to address this requirement. New textbooks should be developed according to the curriculum revision. Especially addressing digital literacy is quite a burden to textbook developers since the strength of emphasis is quite stronger than before. Another domain is school who should operate field education. However, they are not ready for this change in curriculum and school environment is not fully ready for this. Another domain is university, which has potent to help and assist schools and teachers for this goal. Especially university labs have resources and experiences in data based research in science research. These can be helpful to field education. However, linking these two domain is not easy. So collaboratory works and much of considerations are necessary for field schools to deal with this digital literacy at schools.

Symposium : **EDU1-2**
Current Issues and Research in Chemistry Education
Room 304 FRI 09:25
Chair: Wonho Choi (Sunchon National University)

Cases and Suggestions for General High School Chemistry Classes to Cultivate Students’ Competencies in the High School Credit System of the 2022 Revised Curriculum

Saetbyeol Moon

Buyeong Girls' High School, Korea

The 2022 revised science curriculum aims to foster talented people with scientific knowledge that can flexibly respond to the future society that creates a convergence area based on advanced science and technology. Accordingly, the class was structured to utilize an artificial intelligence data analysis program to understand chemistry principles, and the two aspects of AI as a teaching and learning tool and AI as educational content were taught through the class. Supervised learning and unsupervised learning were performed based on various data on elements. Through this result, the reason for the periodic nature of the element was found and the trend was visually understood.After class, students said that activities using artificial intelligence tools helped them understand chemical concepts and that they wanted to use artificial intelligence in other concepts or other subjects. In addition, the proportion of students who have confidence in using artificial intelligence tools and think positively has increased.Since students' thinking and competence are changed by education, teachers should make efforts to improve their expertise in utilizing edutech, develop class design and evaluation models using digital tools, and share the examples. The College of Education should open various educational programs and support regular training. The Ministry of Education and the Metropolitan Office of Education should create an edutech environment by establishing a stable wireless network and supporting one laptop per person. If teachers' ability to use EduTech and an environment to express it are prepared, students will be able to cultivate digital literacy along with core competencies in various online and offline classroom environments with the high school credit system.

Symposium : **EDU1-3**

Current Issues and Research in Chemistry Education

Room 304 FRI 10:10

Chair: Wonho Choi (Sunchon National University)

Changes in the evaluation system of Daejeon science high school as a case of evaluation in the 2022 revised curriculum.

Mi Young Han

Department of Chemistry, Daejeon Science High School for the Gifted, Korea

The evaluation system in 2022 revised curriculum is changed from relative 1~9 grade evaluation to absolute evaluation. Moreover the total instructional hours and credit per subject are reduced, and the diverse elective subjects are provided in line with the purpose of the high school credit system. In the first grade students take common mandatory subjects and are allowed to select the subjects in general/career/convergence electrive subjects for their career plans and aptitude.This change is very similar to the change in the curriculum and evaluation of Daejeon Science High School, which has been converted into a gifted school for 10 years. In Daejeon science high school, students take common mandatory subjects in the first grade, and then select subjects in the basic/advanced/convergence elective subjects in the secone and third grade according to their career plan and aptitude. For evaluation system, it was changed from absolute evaluation to relative evaluation, but now only AP subjects maintain relative evaluation, other subjects are converted to absolute evaluation. In addition, all subjects are planned to converted to absolute evaluation from 2025. In this process various advantages and disadvantages of each evaluation system were revealed. This trial and error is a pilot case that can show problems that could appear in evaluation system in the high school credit system.In 2015, Daejeon science high school changed the absolute evaluation to relative evaluation except the basic subjects such as Korean, English, Society. It was because to solve the problems that occurred in the absolute evaluation. The difference in distribution of graeds between subjects was occurred by the difference in achievement standards not by the difference of absolute achievement of each student. Especially, students complained that what subject they choose, not an individual's academic achievement, determines the grade. However, in the relative

evaluation, even though students' achievement levels are similar in subjects with fewer than 10 students, the relative grade should have been evaluated. As a result, minority subjects and convergence subjects were changed to absolute evaluation again, and now absolute evaluation are applied to all subjects to the first grade of 2023. However, the problems of absolute evaluation is still emerging. The difference of grade distribution in the same elective subjects group often affects the selection of subjects by student and expressed as a official complaint. The inter-subject communication and discusstion for the achievement standard are very needed to absolute evaluation system.

Symposium : **EDU1-4**

Current Issues and Research in Chemistry Education

Room 304 FRI 10:35

Chair: Wonho Choi (Sunchon National University)

The characteristics of understanding about chemistry: Focusing on the results of the National Assessment of Educational Achievement(NAEA) and Customized Assessment for Educational Achievement(CAEA)

Jongho Baek

Korea Institute for Curriculum and Evaluation, Korea

National Assessment of Educational Achievement(NAEA) is a large-scale assessment conducted for examining students' understanding about national curriculum. Recently "Customized Assessment for Educational Achievement"(CAEA) introduced to support teaching and learning by providing customized results of assessment for individual students, unlike the NAEA. NAEA is conducted by sampling 1.5% of third grade middle school students in Korea, while the CAEA is conducted on a class which registered by each school. In addition, the CAEA is characterized that it targets elementary school students to middle school students. The purpose of this study is to examine the characteristics of understanding about chemistry by analyzing the results of NAEA and CAEA during the 2015 revised curriculum. In this presentation, results of NAEA covers the first semester of middle school through the first semester of third grade. The results of CAEA which are analyzed in this study are from the second semester of fifth grade to the first semester of sixth grade of elementary school. Based on the results of analysis, this presentation will include the discussion for teaching and learning by examining specifically students' understanding of chemistry.

Symposium : **EDU2-1**
Chemistry Education for the Science Gifted Students
Room 304 FRI 14:30
Chair: Kihyang Kim (Sejong Academy of Science and Arts)

Development and application of science gifted education programs using maker education: Focusing on chemical cell

Nowon Park

Department of Chemical Education, Gyeonggi Science High School for the Gifted, Korea

In this study, we developed a regular curriculum program for science gifted students by applying maker education that is suitable for developing competencies required in the future, such as problem-solving, collaboration, and communication skills. We also aimed to explore the effectiveness and implications of introducing maker education into the regular curriculum of science gifted schools by applying the developed program.In order for a chemical cell to work effectively, a program was developed to explore how each component of the cell affects the performance of the chemical cell. We measured the voltage and current of a chemical cell while manipulating variables expected to affect the cell's performance, such as the type and area of metal plates used as electrodes, the distance between metal plates, and the type and concentration of electrolyte. They built maker devices appropriate for checking the effects of each variable, and based on their findings, they designed a program to devise a device that can physically compute the performance of a cell.The developed program was applied to 26 students at G Science Gifted School in Gyeonggi-do for six sessions, and data such as student activity sheets and teacher observation records, class transcriptions based on class activity recordings, and interviews with some students after the program was applied were collected during the research process. To analyze the degree of expression of maker competencies, we analyzed the verbal interactions of students in class activities and conducted a triangulation analysis of various types of data to check the educational effectiveness of the program.As a result, the degree of expression of maker competencies was compared to previous studies on middle school science gifted students, and the frequency of expression of each competency group was similar in the order of 'collaboration' > 'making' > 'integrative thinking' > 'maker mind' > 'problem discovery' >

'human-centeredness'. As a result, the frequency of expression of each maker competency group was in the order of 'collaboration' > 'making' > 'integrative thinking' > 'maker mind' > 'problem finding' > 'human-centeredness', which was similar to the results of previous studies. However, when we analyzed the characteristics of science gifted students more closely by core competencies, we found that 'intuitive thinking' and 'communication' competencies appeared in large numbers. When we specifically compared this to previous studies of middle school science gifted students, we found that the "intuitive thinking," "sharing," and "communication" competencies were about twice as prevalent, while the "enjoyment of the making process" competency was less than half as prevalent. It was analyzed that the main reason for this difference was the prevalence of 'intuitive thinking'. It was repeatedly observed that when there were not enough observations to logically explain the phenomenon in the inquiry activity, students expressed a lot of "intuitive thinking" followed by "communication" and "sharing" to explain its validity. On the other hand, in situations where there were many tasks to be performed to reach the goal of the lesson, it was found that the 'enjoyment of the making process' was less expressed as the maker activity itself was perceived as a means rather than an end due to the burden of achieving the tasks. Interviews with students after the program confirmed that maker activities can partially change students' tendency to rely on tools in measurement activities, and that there are educational effects such as deeper understanding of course content, increased teacher-student and student-student communication, and positive perceptions of collaboration. However, we also found that there were some negative feelings about the inaccuracy of the maker devices and the time required to make the devices, which hindered their exploration. Therefore, to improve the effectiveness of maker education, it is necessary to improve the accuracy of the maker devices and to provide appropriate guidance strategies for the content and time of each step in teaching and learning activities.The significance of this study is that it developed an educational program for high school science gifted students to apply maker education as a regular curriculum activity, and suggested teaching and learning methods according to the characteristics of students, and suggested ways to refine teaching and learning methods to apply maker education to regular curriculum classes.

Symposium : **EDU2-2**

Chemistry Education for the Science Gifted Students

Room 304 FRI 15:00

Chair: Kihyang Kim (Sejong Academy of Science and Arts)

Normal Chemistry Class

Daeseong Jin

Department of Chemistry, Daejeon Science High School for the Gifted, Korea

I have designed my chemistry class using the Process-Focused Assessment for 2 years. I had my students think more deeply about chemical phenomena. I chose some pictures from a chemistry text book, and I had the students look into the pictures to find any problems or questions. Then the students discussed the problem each other. The aim of this class is to improve critical science thinking and cooperative ability.

Symposium : **EDU2-3**
Chemistry Education for the Science Gifted Students
Room 304 FRI 15:30
Chair: Kihyang Kim (Sejong Academy of Science and Arts)

A meeting chance for gifted science students! Introducing international science festival for science gifted students - Focusing on KSASF 2023

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

What is a meeting chance for science gifted students? The research paper and research conferences provide the chance to scientists not only to share their research results but also to learn research trends and new ideas. Science gifted students who want to be the future scientists also need this kind of meeting chances. Korea Chemical Society Meeting gives such a chance to science gifted students who want to be future chemists. However, it is necessary for science gifted students not only to share the results of their research activities, but also to experience science projects together and enjoy together.The international science festival for science gifted students introduced in this presentation provides a meeting chance for science gifted students to work together and learn from each other. I Introduce the KSASF program of the Korea Science Academy which is one of international science festival for science gifted students, which was first conducted offline after COVID-19. The KSASF 2023 science festival was held from July 27th to July 30th at Korea Science Gifted School in Busan. The KSASF 2023 science festival presents 'Science and the Future' as the main theme along with the slogan "Explore the Horizon," and is a program that reflects convergent thinking and technologies such as environment-energy, bio-, nano-, and space science, and information and communication. It provided opportunities for gifted science students to communicate through science and grow through imagination, ideas, and spirit of challenge.It is expected that the opportunity to participate in the international science festival will provide science gifted students with an opportunity to communicate and grow together as future global leaders.

Symposium : **EDU2-4**

Chemistry Education for the Science Gifted Students

Room 304 FRI 16:00

Chair: Kihyang Kim (Sejong Academy of Science and Arts)

The Effect of the Chemistry Experiments Utilizing Advanced Laboratory Equipment of Science High School on the Affective Characteristics in Science Aspect of Ordinary High School Students

Jihun Park

Busan Science High School, Korea

This research is conducted to investigate the effect of the chemistry experiment classes utilizing advanced laboratory equipment of science high school on the change of ordinary high school students' affective characteristics in science aspect. For this purpose, we have developed six new courses relying on advanced laboratory equipment such as UV-VIS spectrometer and NMR. Also, pre- and post-test surveys about affective characteristics of students, post-program survey and interview materials were collected and analyzed. As a result, we did confirm the significant effect of those courses on ordinary high school students' affective characteristics. By operating the advanced laboratory equipment and experimenting with it, The students could have a variety of experiences related to careers that they could rarely have in ordinary high school. Further, it is shown that various chemical experiences through professional experiment activities beyond repeated question solving focused on exams have exerted influence on the change in the perception of chemistry. Unfortunately, such chemical experiments within the current curriculum can be achieved only through extra curricular programs or special lectures held during vacation. In that respect, this research can give us the significant implications for subject organization or operation through the development of co-operated curriculum.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ENVR1-1**

Micro- and Nanoplastics: Up-to-date Knowledge on Detection and Toxicity

Room 301 THU 15:40

Chair: Eun-Ju Kim (KIST)

Advancing Raman Spectroscopy for Nanoplastic Detection

Dongha Shin

department of chemistry, Inha University, Korea

Recently, there has been a growing interest in nanoplastics, but measuring them non-destructively is still a challenge. Our presentation will discuss an efficient method for analyzing nanoplastics using Raman spectroscopy and its potential applications in various situations.

Symposium : **ENVR1-2**
Micro- and Nanoplastics: Up-to-date Knowledge on Detection and Toxicity
Room 301 THU 16:10
Chair: Eun-Ju Kim (KIST)

Photooxidation-induced weathering and fragmentation of plastics: from macro to nanoplastics

Young Kyoung Song

Chonnam National University, Korea

Microplastics are widespread in the environment, formed through the gradual weathering and fragmentation of larger plastics into nanoplastics (NPs) and microplastics (MPs). However, the weathering process and fragmentation rate remain poorly understood. To address this, we measured the size distribution of NP and MP particles from expanded polystyrene (EPS) under sunlight exposure. We also examined virgin and additive-containing polypropylene (PP) sheets in a simulated sunlight chamber, followed by mechanical abrasion. The 50% weight loss of an EPS cube due to sunlight weathering is estimated to occur over a span of 3.5 years, and approximately 2.6 x 10^8 particles/cm^2 of fragmented particles could be produced in a single year through sunlight exposure. Many EPS debris items directly exposed to sunlight can rapidly generate numerous micro- and nano-sized particles. The fragmentation rate of PP and PPa (additive-containing PP) appeared similar after 176 days of simulated sunlight exposure followed by mechanical abrasion (equivalent to 2.7 years of outdoor exposure in the Republic of Korea). When examining the quadratic regression graphs for PP, depicting the correlation between total particles produced and exposure duration, PP's fragmentation rate might surpass PPa's after a specific period of sunlight exposure (e.g., 2.7 years). Additionally, we observed that mechanical stress from vortexing played a significant role in the production of MPs, whereas it had a smaller impact on the generation of NPs. This study offers critical insights into plastic weathering and fragmentation processes, paving the way for further investigations into the environmental consequences of NP and MP generation, as well as the potential impacts of plastic additives on these mechanisms.

Symposium : **ENVR1-3**

Micro- and Nanoplastics: Up-to-date Knowledge on Detection and Toxicity

Room 301 THU 16:40

Chair: Eun-Ju Kim (KIST)

Size effects of microplastics with PAH on cardiotoxicity in zebrafish larvae

Jinyoung Jeong

Environmental Disease Research Center, KRIBB, Korea

Microplastics, small plastic particles less than 5 mm generated from plastic debris, have an affinity with various environmental pollutants such as heavy metals, polycyclic aromatic hydrocarbons (PAHs), pesticides, and pharmaceuticals. Among them, PAHs are representative organic contaminants which can absorb on surface of hydrophobic microplastics and transfer to organisms leading potential toxic effects. However, there are many factors to influence the combined toxicity of PAHs and microplastics. In this study, we investigated the size effect of microplastics in presence of PAHs by co-treatment of three different sized polystyrene microplastics and benz[a]anthracene(BaA) in zebrafish embryos. The cardiotoxicity induced by BaA were observed to be accelerated with small sized PSMP (0.2 µm) in contrast to be alleviated with large sized PSMP (10 µm). It was found that the body burden of BaA with PSMP (0.2 µm) was higher than that with PSMP (10 µm) in zebrafish larvae, resulting in increased ROS, cell death in the heart, and eventually heart defects. This results demonstrated that small microplastics could deliver environmental pollutants into the organisms and cause combined toxicity by the trojan-horse effects.

Symposium : **ENVR1-4**

Micro- and Nanoplastics: Up-to-date Knowledge on Detection and Toxicity

Room 301 THU 17:10

Chair: Eun-Ju Kim (KIST)

Fate and Effect of Microplastics in the Soil-plant System

Hakwon Yoon

Environmental Exposure & Toxicology Research Center, Korea Institute of Toxicology, Korea

Recently, the environmental and agricultural impact of plastic waste has attracted considerable attention. Especially, large amounts of micro- (MPs) and nanoplastics(NPs), which are released into the environment through environmental weathering of plastic items or sludge disposal/application, can end up in the soil, being considered as a new plant abiotic stressor. Here, we show that smaller, fragmented NPs can accumulate in the root of Arabidopsis thaliana under combined NPs and Cd stresses. The specific changes in root exudation of organic acids and bacterial community composition that reveal a metabolic preference for aromatic compounds drive the degradation of NPs in the rhizosphere. Additionally, we investigated the impact of sub-micron polyethylene and polypropylene MPs on nitrogen cycling, with an emphasis on bacterial abundance and diversity in a soil-soybean system. Exposure to soil containing MPs did not affect soybean growth, but significantly increased plant nitrogen uptake, which was confirmed by increased activities of nitrogenase in the soil and glutamine synthetase in soybean root. MP also stimulated nitrogen cycling in the soil-legume system and increased the total nitrogen content of soybean, which could be attributed to changes in the abundance and activity of rhizosphere bacteria, as evidenced by an increase in the copy number of 16S rRNA genes and utilization of carbon and nitrogen substrates. Our findings provide critical implications relevant to food security that nanoplastics will contaminate crops as well, and in turn, transfer along the human food chain. Additionally, these results provide insights into the interactions between MPs and rhizosphere bacterial communities in the soil-legume system.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Symposium : **ENVR2-1**
CCU Alchemist Technologies: Carbon-to-Liquid
Room 301 FRI 09:00
Chair: Hyunwoong Park (Kyungpook National University)

Break-Through Technology for the Highly Efficient CO2 Conversion into Solar Liquid Fuels

Young soo Kang

Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

Global warming is one of the serious environmental issues that creates many disasters, including heat waves, floods, storms, and droughts. [Ref 1] Among some greenhouse gases in the atmosphere, CO2 is considered as one of the most critical climate change gas. Photoelectrochemical (PEC) and photocatalytic CO2 conversion into fuels by solar light are simple and effective method to reduce and convert CO2 gas to overcome global warming issues marginally. In this work, multi-layered hybrid composite catalysts have been prepared to be used as catalytic system and devices. This is new and break-through pioneering to have sequential multi-electron shuttling function to produce liquid fuels, reduction potential tuning for product selectivity, CO2 activation to reduce CO2 conversion reaction energy and activation energy and different multi-electron/proton transport pathway. rGO has been used for multi-electron shuttling functional layer. Poly(4-vinyl)pyridine has been selected to adsorb and activate a highly stable CO2 molecule. Different electron/proton transport pathway has been fabricated by separating the porous conducting carbon based polymer backbone by attaching -SO3- functional group on the inner and outer sides of the porous carbon backbone in the case of photocatalytic system and fabrication two different pathway of electron with external wire and proton conducting Nafion layer on the opposite side of cathode in the case of PEC system. The structure of hybrid composite was confirmed by XRD and XPS, thickness of each layer was observed by SEM cross-section image. Electrochemical properties of each layer were studied and investigated by LSV, CV and EIS. Products analysis was carried out with Gc, GC-MS and NMR.

Symposium : **ENVR2-2**

CCU Alchemist Technologies: Carbon-to-Liquid

Room 301 FRI 09:20

Chair: Hyunwoong Park (Kyungpook National University)

Mesoporous Zeolite Supported with Metal Catalysts for CO_2 Conversion to Methanol

Ryong Ryoo

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

Numerous processes for removing carbon dioxide have been studied to solve the greenhouse effect, and CO_2 hydrogenation to methanol is a very promising process among them because of the industrial value of methanol. However, the catalytic activity of this reaction has been suppressed due to the high structural stability of CO_2 , necessitating substantial improvements. To enhance the catalytic performance of traditional catalysts like copper (Cu) and palladium (Pd), researchers have explored about additional promoters such as indium (In). The metal catalysts with promoters have exhibited improved performance by generating oxygen vacancies, but the problem about encapsulation and deactivation of catalyst due to the strong metal-support interaction of oxide has acted as a major challenge to use alloy as a catalyst for the CO_2 conversion to methanol.Recently, our group reported a novel approach about platinum-rare earth element alloy catalysts synthesized on the surface silanol of mesoporous zeolite. The presence of surface silanol facilitates the atomistic diffusion of rare earth element to form the intermetallic structure with platinum, thus it was possible to yield alloy nanoparticles of them. This nanostructured catalyst has shown remarkable catalytic performance in the propane dehydrogenation reaction. In this perspective, we extended our investigation to prepare alloy nanoparticles of palladium and indium supported on the mesoporous zeolite, for catalyzing CO_2 conversion to methanol reaction. Notably, this alloy nanoparticle catalyst has shown improved CO_2 conversion and methanol selectivity compared to previously reported activities. Furthermore, our research has been extended to the exploration of various metal-indium alloy catalysts supported on mesoporous zeolite.

Symposium : **ENVR2-3**
CCU Alchemist Technologies: Carbon-to-Liquid
Room 301 FRI 09:45
Chair: Hyunwoong Park (Kyungpook National University)

Gas Separation Using Membrane Contactor and Application

Joonwoo Kim

Research Institute of Industrial Science & Technology, Korea

In order to meet the NDC 40%, which is the carbon-neutral goal of Korea, it is necessary to use a negative strategy that captures and utilizes CO2 in air as well as CO2 from point sources. Conventional CO2 capture technology requires a large amount of energy during regeneration, which leads to CO2 emission. However, since membrane contactor technology uses power-based regeneration technology, it can be a good alternative to existing technology when linked with renewable energy. In addition, in conjunction with aqueous solution-based photoelectrochemical technology, it can be directly utilized without the additional energy of CO2 extraction. In this study, we would like to introduce various applications of membrane contactor technology and CCU technology using CO2.

Symposium : **ENVR2-4**
CCU Alchemist Technologies: Carbon-to-Liquid
Room 301 FRI 10:00
Chair: Hyunwoong Park (Kyungpook National University)

Membrane-based greenhouse gas capture from fossil fuel flue gas

Hyo Won Kim

Department of Energy Engineering, Korea Institute of Energy Technology, Korea

Carbon dioxide (CO2) capture plays a crucial role as a fundamental technology in the quest for carbon neutrality. This is because petrochemical systems, which emit CO2 during their processes, remain the primary means of producing valuable chemicals, fuels, and energy sources. Specifically, the combustion of fossil fuels has been considered as a key process releasing CO2 alongside steam, another greenhouse gas. Consequently, it becomes imperative to effectively separate both CO2 and water vapor from the mixture found in flue gas.However, there are currently no methods available to capture both gases simultaneously, underscoring the need for the development of novel approaches to extract them from flue gas. We here introduce a fresh conceptual framework that leverages polymeric membranes developed in our study to transport both plasticizing gases concurrently. To illustrate this concept, we present a CO2 transport employing plasticization-tolerant semi-crystalline polymer materials under humidified conditions.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Symposium : **ENVR2-5**
CCU Alchemist Technologies: Carbon-to-Liquid
Room 301 FRI 10:15
Chair: Hyunwoong Park (Kyungpook National University)

Electrochemical CO2 reduction reaction at zero-gap membrane electrode assembly

Yun Jeong Hwang

Chemistry Department, Seoul National University, Korea

The need to develop carbon capture and utilization (CCU) technology has been sharply emerging due to the global agenda to achieve carbon neutrality. Electrochemical CO2 reduction (CO2R) can be integrated with renewable energy sources and water can be utilized as a direct proton source which is promising to provide a sustainable carbon cycle. However, CO2R to useful carbon chemicals is challenging to meet the industrial requirements. Recent studies on electrocatalysts and systems have made a significant improvement in the performances both of product selectivity and current density, but many underlying phenomena are still not clearly understood. Gas-diffusion electrode configurations allow direct CO2 gas-feeding to the catalyst layer and several hundred mA/cm2 of current density have been demonstrated with a zero-gap type of membrane electrolyzer assembly (MEA) electrolyzer. Among various components of MEA, here, I will focus on the cathode catalyst and balanced CO2 and water supply at the catalyst/membrane boundary. CO2 and water supply is important factor in tuning the activity/selectivity since CO2R is sensitively affected by mass transport. In addition, we confirmed the importance of cathode catalyst porosity for CO2R in the zero-gap MEA electrolyzer to achieve high current density. These studies will give insight into the intrinsic and extrinsic factors to achieve selective CO2R to target products and can contribute to demonstrating more practical applications.

Symposium : **ENVR2-6**

CCU Alchemist Technologies: Carbon-to-Liquid

Room 301 FRI 10:30

Chair: Hyunwoong Park (Kyungpook National University)

Electrochemical Carbon-to-Liquid Technologies

Ki Tae Park

Konkuk University, Korea

The electrocatalytic CO2 reduction reaction (CO2RR) to liquid products has gained significant attention as a potential environmentally friendly approach to reducing CO2 emissions and producing carbon-neutral liquid fuels. There are two pathways of one-step and multi-step reaction processes to produce liquid products from CO2. Liquid products containing one or two carbons, such as formic acid and methanol, can be directly produced through electrocatalytic CO2 reduction reactions (CO2RR) with high selectivity. However, liquid fuels with higher carbon content, like gasoline or diesel, require additional catalytic reaction processes that utilize intermediate feedstocks such as syngas or alcohols generated from CO2RR processes. The present study introduces recent research findings on CO2RR to produce formic acid, which recently has received significant interest as a liquid fuel and hydrogen carrier, as well as CO2RR research for the production of syngas, a reactant for Fischer-Tropsch (FT) synthesis reactions used in the production of multi-carbon liquid fuels.

Symposium : **ENVR2-7**

CCU Alchemist Technologies: Carbon-to-Liquid

Room 301 FRI 10:45

Chair: Hyunwoong Park (Kyungpook National University)

A Technical Progress Towards Artificial Photosynthesis Factory

Hyunwoong Park

School of Energy Engineering, Kyungpook National University, Korea

As the cost of carbon-intensive fuels continues to fluctuate and atmospheric carbon dioxide concentrations rise, there is a growing interest in solar fuels as a clean energy alternative. These fuels include molecular hydrogen and hydrogen peroxide produced from water, as well as hydrocarbons converted from carbon dioxide. In order to achieve high-efficiency solar fuel production, it is not only important that light absorbers absorb most sunlight, but also that charge separation and interfacial charge transfers occur efficiently. There has been renewed interest in recent years in the photocatalytic and photoelectrochemical conversion of CO2 into value-added chemicals using various semiconductor particles and electrodes. While the production of C1 chemicals in aqueous media is common in CO2 reduction, the production of C2-C4 hydrocarbons has also been reported. Many photocatalytic materials have been studied, but they still suffer from low selectivity, poor energy efficiency, and instability, while also failing to drive simultaneous water oxidation. In this talk, I will present recent studies of my group on solar CO2 conversion to value-added chemicals using water as an electron donor in various photo-systems

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 09:00

Chair: Jeung Gon Kim (Jeonbuk National University)

Fast and Large Motion of Self-Oscillating Gels based on High Diffusivity Induced by Phase-separated Structures

Jaewon Choi, Taehun Chung, Ryo Yoshida[1], Younsoo Kim*

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

[1]*Department of Materials Engineering, The University of Tokyo, Japan*

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, 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.

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 09:12

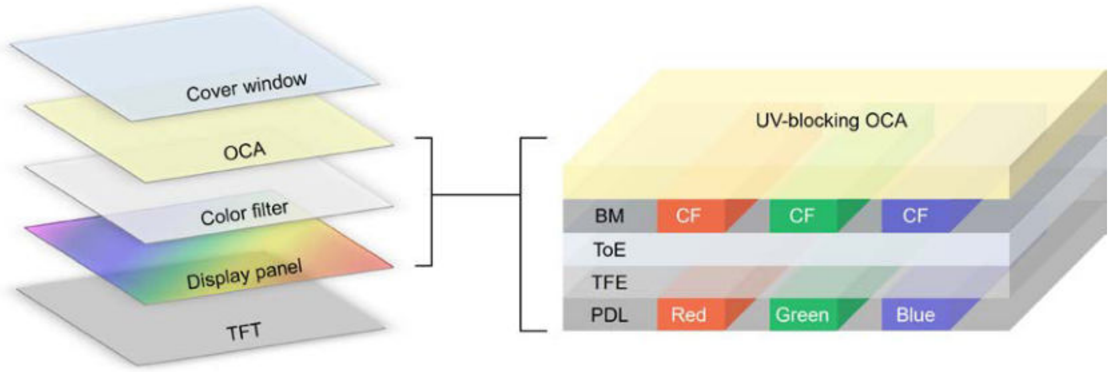
Chair: Jeung Gon Kim (Jeonbuk National University)

Ultraviolet Light Blocking Optically Clear Adhesives for Foldable Displays via Highly Efficient Visible-Light Curing

Seokju Lee

Materials and science engineering, Seoul National University, Korea

To reduce power consumption, the design of a new foldable smartphone's organic light-emitting diode (OLED) panel necessitates the utilization of an advanced, optically transparent adhesive (OCA) capable of blocking UV light, in addition to its conventional functions of adhesion and strain relief. However, conventional UV curing methods cannot be used to prepare UV-blocking OCA due to the UV-blocking agent’s high absorbance of UV light. Recently, a method for producing UV-blocking OCA through visible-light curing has been proposed, utilizing a new photo-initiating system (PIS). Nevertheless, the curing speed remains significantly slow, which hinders its commercialization. In this study, we have developed a highly efficient photo-initiating system (PIS) that enables the rapid production of UV-blocking OCAs suitable for commercialization under visible-light irradiation. By analyzing existing PISs, we identified triplet-triplet energy transfer as the main factor hindering the curing rate. To address this, we used a newly designed photocatalyst (PC) with a lower energy transfer rate to UV absorbers compared to the previous PC. Combining the PC with carefully chosen co-initiators, we created a new PIS that generates radicals rapidly through electron transfer. Under 452 nm visible light, we achieved UV-blocking OCAs at a rate approximately 10 times faster than before, while maintaining excellent UV-blocking ability and optical transparency. In UV-blocking tests, our OCA-covered OLED device demonstrated superior UV-blocking performance, indicating broad applications in protecting diverse smart devices with various form factors from UV irradiation.*Yonghwan Kwon,*[†] *Seokju Lee,*[†] *Min Sang Kwon*[*]


Cover window
OCA
Color filter
Display panel
TFT
UV-blocking OCA
BM
CF
CF
CF
ToE
TFE
PDL
Red
Green
Blue

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 09:24

Chair: Jeung Gon Kim (Jeonbuk National University)

Vertically oriented Ti3C2Tx MXene nanosheets for electromagnetic wave control

Changjae Lee, Dong Ki Yoon*

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

The inherent anisotropy of two-dimensional (2D) nanomaterials, characterized by their high aspect ratio, provides excellent opportunities for achieving directional functionality. Specifically, the edge of 2D titanium carbide, Ti3C2Tx MXene (Tx= O, OH and F), is theoretically predicted to show a huge difference in light absorbance depending on the incident polarization direction in the long-wavelength range. However, this phenomenon has not been experimentally demonstrated, as it is challenging to uniaxially orient the MXene edges in a sufficiently large area. Here, we demonstrate the utilization of vertically aligned Ti3C2Tx MXene with a significant content of oriented edges as a linear polarizer in the terahertz (THz) frequency region. By exploiting the high surface charge and excellent colloidal dispersibility of MXene nanosheets, we rationalize the MXene THz polarizer based on vertically oriented MXene nanosheets along an applied alternating-current electric field in an aqueous solution. Our polarizer exhibits exceptional performances, including a notable extinction ratio exceeding 12 dB, which is twice as high as that of previously reported MXene-based THz polarizer, along with an optimal insertion loss below 5 dB. In addition to the simple uniaxial arrangement, a radially patterned polarizer is developed in a designed circular electrode cell to implement spatially different polarizations in one sample. Our results represent a significant advancement in the optical utilization of vertical 2D materials, offering new possibilities for their potential applications.

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 09:36

Chair: Jeung Gon Kim (Jeonbuk National University)

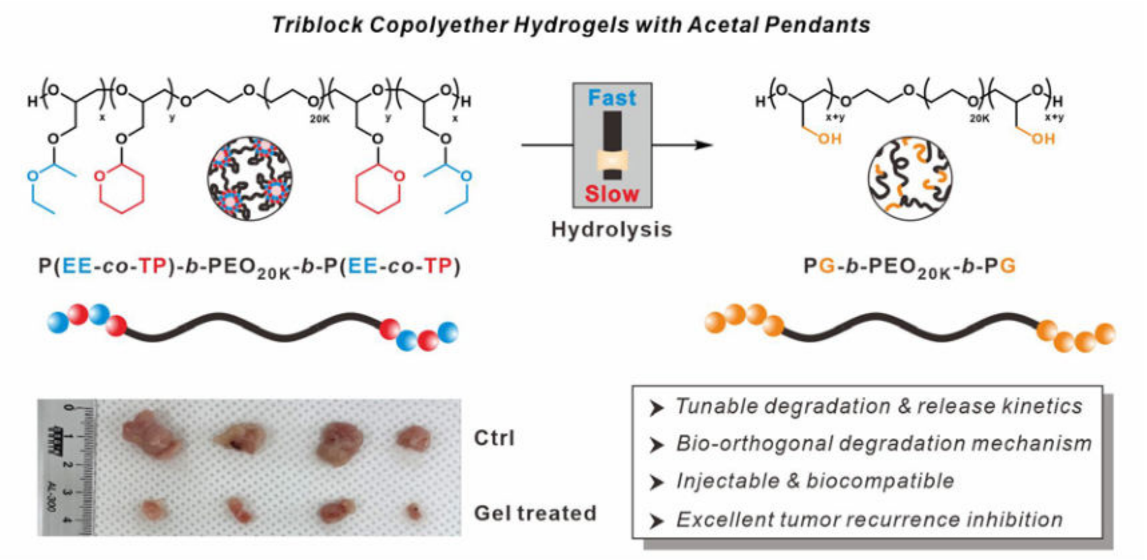
Highly Tunable Mechano-Temporal Profiles in Triblock Copolyether Hydrogels with Mixed Acetal Pendants

Jinsu Baek, Byeong-Su Kim[1,*]

Department of chemistry, Yonsei University, Korea

[1]Department of Chemistry, Yonsei University, Korea

While dual pH-thermo-responsive hydrogels have been extensively studied in the biomedical field, precise control of degradation and release kinetics still remain a challenge. In this study, we introduce a series of poly(ethylene oxide)-based ABA triblock hydrogels with varying ratios of labile ethoxyethyl (EE) and stable tetrahydropyranyl (TP) hydrophobic acetal on the A block. This approach allows the hydrogel to cover a wide spectrum of hydrolysis kinetics under mild acidic conditions, without compromising its crosslinking density or stiffness. Notably, the hydrogel's ability to gradually release the micelles with a hydrophobic dye further provides the protection of loaded molecules from enzymes or proteins after being released from the hydrogel. Additionally, our unique hydrogel platform shows that it can effectively suppress the tumor recurrence after resection, highlighting the potential for versatile applications especially which requires a precise control of the degradation and release kinetics. Overall, this novel pH-responsive hydrogel presents a promising platform for various biomedical applications.


Triblock Copolyether Hydrogels with Acetal Pendants
x
y
20K
y
x
Fast
Slow
Hydrolysis
x+y
20K
x+y
OH
OH
P(EE-co-TP)-b-PEO20K-b-P(EE-co-TP)
PG-b-PEO20K-b-PG
Ctrl
Gel treated
Tunable degradation & release kinetics
Bio-orthogonal degradation mechanism
Injectable & biocompatible
Excellent tumor recurrence inhibition

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 09:48

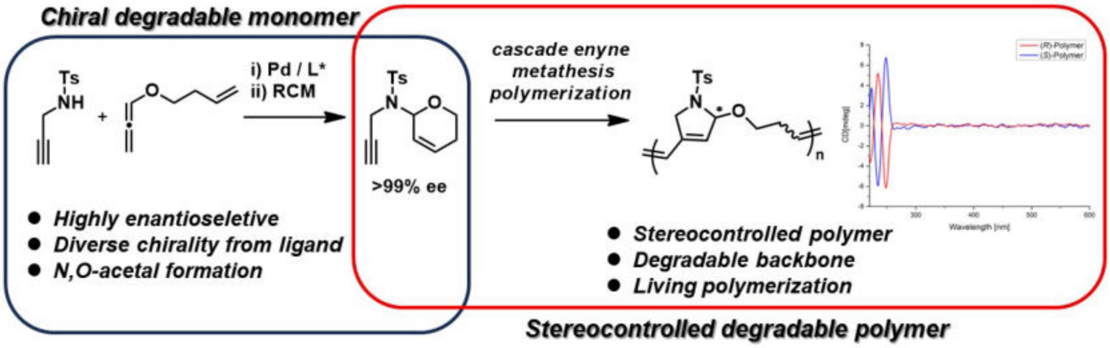
Chair: Jeung Gon Kim (Jeonbuk National University)

Synthesis of stereocontrolled *N*,*O*-acetal-containing polymer by cascade enyne metathesis polymerization

Bon Woo Koo, Cheoljae Kim*

Department of Chemistry, Chungbuk National University, Korea

We have precisely synthesized stereocontrolled polymers from enantiomerically pure *N*,*O*-acetal-containing enyne monomers by cascade enyne metathesis polymerization. Chiral acetal-containing enyne monomers were prepared by asymmetric hydroamination of alkoxyallene with chiral Pd catalyst and following ring-closing metathesis. Due to the acetal moiety in the polymer backbone, the obtained polymers were degraded under acidic media. We also synthesized various di- and tri-block copolymers from degradable and non-degradable enyne monomers as well as norbornene. Additionally, the postmodification of the polymers was proceeded by aza-Diels-Alder reaction.


Chiral degradable monomer
Ts
NH
+
O
i) Pd / L*
ii) RCM
Ts
N
O
>99% ee
Highly enantioseletive
Diverse chirality from ligand
N,O-acetal formation
cascade enyne metathesis polymerization
Ts
N
O
n
(R)-Polymer
(S)-Polymer
CD [mdeg]
Wavelength [nm]
300
400
500
600
Stereocontrolled polymer
Degradable backbone
Living polymerization
Stereocontrolled degradable polymer

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 10:00

Chair: Jeung Gon Kim (Jeonbuk National University)

Chain Length-dependent Deoxygenation of Polyacrylate for Synthesis of Functional Polypropylene

Seongjang Jeon, Taeseok Oh, Myungeun Seo[*]

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

The reactivity of functional groups attached to polymers is generally assumed to be similar to that of low-molecular-weight homologs if the condition is identical. The solubility of reactants and products in reaction media should not be changed during the reaction. Only the individual functional groups are involved in the reaction. And the steric factor must be similar. However, for many reasons, the reaction of polymers is usually observed with low conversion and reaction rate or vice versa, which is affected by concentration, crystallinity, changes in solubility, and neighboring group effect. Here we explore a case of a catalytic reaction whose rate depends on the chain length of the polymer substrate. With the increasing chain length, i.e., degree of polymerization (DP), the reaction rate decreases initially but increases above a critical number. We posit that binding of the catalyst to the reacting motifs densely distributed along the polymer chain would be sterically less favored over a small molecular system. This unique pathway is demonstrated with borane-catalyzed deoxygenation of poly (methyl acrylate) using hydrosilane as a reducing agent, which eliminates oxygen atoms in the pendant and produces polypropylene. This post-polymerization defunctionalization route allows us to produce polypropylenes with very high yet controllable functional group loading, as we start from the 100% functionalized.

Oral Presentation : **POLY.O-7**
Oral Presentation for Young Polymer Scientists
Room 302+303 THU 10:12
Chair: Jeung Gon Kim (Jeonbuk National University)

SIMPLIFIED Y6-BASED NONFULLERENE ACCEPTORS: IN-DEPTH STUDY ON MOLECULAR STRUCTURE–PROPERTY RELATION, MOLECULAR DYNAMICS SIMULATION, AND CHARGE DYNAMICS

Minhun Jee, Sungnam Park*, Han Young Woo*

Department of Chemistry, Korea University, Korea

In organic solar cells, Y6 derivatives have emerged as promising candidates due to low energy loss with a notable electroluminescent quantum efficiency, a dominant face-on orientation, and high electron mobility. However, the complex and long synthetic process required to synthesize BTP core for Y6 derivatives presents a significant challenge. To address this, we synthesized two novel Y6 derivatives, named YBO-2O and YBO-FO. This design incorporates a simplified synthetic procedure by repositioning the alkyl substituents responsible for solubility on the BTP core to the terminal INCN groups. The removal of bulky alkyl side chains from the core led to a reinforcement of intermolecular packing compared to Y6, and this enhancement was verified through molecular dynamics (MD) simulations. The outcomes revealed that both YBO-2O and YBO-FO exhibited a more compact core-core and terminal-terminal (CC-TT) packing arrangement compared to Y6. This observation correlates with results obtained from GIWAXS, indicating tighter packing, and SCLC measurements, indicating enhanced electron mobility in YBO-2O and YBO-FO. Furthermore, the introduction of the electron-donating terminal group (INCNO2) led to an elevation in the HOMO and LUMO energy levels of YBO-2O and YBO-FO. Notably, YBO-FO displayed a HOMO energy level compatible with that of the polymer donor PM6, promoting efficient hole transfer at the interface between the donor and acceptor materials. In blend films, the process of hole transfer from YBO-2O and YBO-FO to PM6 was analyzed through transient absorption spectroscopy (TAS), revealing a proficient hole transfer from YBO-FO to PM6. Impressively, despite the simplified synthesis route, YBO-FO demonstrated a power conversion efficiency of 15.01%.

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 10:24

Chair: Jeung Gon Kim (Jeonbuk National University)

Eco-friendly Degradable Organic Electrochemical Transistors for Zero E-Waste Electronics

Hyeonjun Na, Myung-Han Yoon[1,*]

Materials science and engineering, Gwangju Institute of Science and Technology, Korea

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

In this study, we fabricated a disposable organic electrochemical transistor (OECT) device using a bio-degradable substrate made of poly(vinyl alcohol)/poly(acrylic acid) (PVA-PAA) coated cellulose paper which was designed to be consumable by the superworm beetle, Zophobas Morio Analytical techniques such as cross-sectional Scanning Electron Microscopy and Universal Testing Machine were utilized to evaluate the substrate's thickness and mechanical strength. Fourier Transform Infrared Spectroscopy was used to confirm the PVA-PAA coating on the cellulose substrate. The OECT device was assembled using a bio-compatible active layer film made of poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS)/montmorillonite (MMT) composites on a PVA-PAA/cellulose substrate and was later consumed by the superworm, demonstrating the feasibility of creating eco-degradable, disposable OECT devices.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 10:36

Chair: Jeung Gon Kim (Jeonbuk National University)

Superoleophilic Nanocellulose Based Sponge for Nanoremediation of Microplastics

Chandravati Yadav, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Synthetic polymeric produces such as plastics have progressed as a state-of-the-art material that has invigorated modern society with multitude of applications, practically in every sector. Indeed, the ever-increasing reliance on these ingenious materials has propelled the world into a “Plasticene” era. Recently, an invisible portion of plastic, namely microplastics (μPs), are at the forefront of current environmental concerns and has become an ever-growing topic of research. Due to the tiny size and colloidal nature, μPs are hard to capture and can easily be ingested by aquatic organisms causing severe toxicity at both cellular and molecular levels. Hence, in addition to reduce plastic generation and consumption, an environmentally friendly remediation approach to tackle the ever-growing μPs pollution is substantially desired. In the present study, a robust Fe_3O_4-TiO_2 decorated nanocellulose sponge functionalized with hexadecylphosphonic acid (HPA) has been reported as an efficient adsorptive material for nanoremediation of various μPs. An adsorption capacity of higher than 85% has been recorded for both carboxylate-modified and amine-modified polystyrene (PS) and the work is underway to determine its adsorption efficiency for various other kinds of μPs. The mechanism of adsorption of μPs was monitored by fluorescence spectrophotometer, FTIR spectroscopy, kinetic studies, thermal analysis, changes in zeta potentials and FESEM. Based on renewability, and excellent accessibility, extraction efficiency and reusability with expected non-toxic effects the developed adsorbent material paves a broad application prospect in the field of μPs remediation.

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

Oral Presentation for Young Polymer Scientists

Room 302+303 THU 10:48

Chair: Jeung Gon Kim (Jeonbuk National University)

Assistance of Up-Conversion Phosphor in TiO2 to Augment Visible Light Absorption for Water Splitting

Amol Uttam Pawar

Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

Artificial photosynthesis is one of the best ways to produce an environmentally clean and renewable energy source. Several photocatalytic materials with improving its performance have been reported since the last several years [1-3]. In the photoelectrochemical system, solar to fuel production depends upon the nature of photoelectrode. This electrode generates photocurrent, which is responsible for the amount of fuel production and solar to fuel efficiency. Hence, enhancing the photocurrent is one of the most important tasks in the photoelectrochemical system. There are different ways to increase this photocurrent, such as metal doping, homo or heterostructure catalysis combination, use Z scheme material combination etc., to avoid electron-hole recombination and enhance visible light absorption for high current density. Here we are going to introduce up-conversion phosphor material (Y2SiO5:Pr3+) assisted TiO2 photoanode for comparatively higher photocurrent. Phosphor material and TiO2 electrodes have been synthesized by simple hydrothermal methods. The film is prepared on FTO back and forth with phosphor and TiO2 nanorod, respectively. The crystallinity, optical properties and photo-response of prepared films were monitored by XRD, UV-visible as well as PL, and IV curve, respectively.

Award Lecture in Division : **INOR.O-1**

Oral Presentation for Young Inorganic Chemists

Room 211+212+213 THU 09:00

Chair: Kyounghoon Lee (Gyeongsang National University)

Observation of Individual Chemical Reaction in Nanoparticle Catalyst and Cell Membrane using Optical Microscopy

Daeha Seo

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

This presentation introduces the use of optical microscopy to investigate chemical reactions in two contexts: 1) nanoparticle photocatalysts and 2) living cell membranes. In catalyst studies, we harness gold's optical properties to enhance photocatalysis. By illuminating gold-Cu2O nanocatalysts with lasers, we uncover electron-transport pathways at the individual particle level, providing new insights into catalyst kinetics and excitations. This advances our understanding of semiconductor nanoparticles within gold.Shifting to cell biology, single-molecule tracking examines the organization of plasmalemma vesicle-associated protein (PLVAP). We link actin destabilization to changes in the cellular structure, specifically the arrangement of fenestrae. This reveals reduced association kinetics. Utilizing single-molecule measurements, we construct a reaction-diffusion model that accurately reproduces the 2D ultrastructure pattern and association stoichiometry. This approach surpasses static imaging, uncovering hidden cellular properties.In conclusion, optical microscopy proves invaluable for deciphering catalyst and membrane reactions, operating at the single molecule/particle level. These innovative techniques shed light on electron transfers and protein arrangements, offering transformative insights into complex systems. This presentation underscores microscopy's potential in advancing chemical biology.

Award Lecture in Division : **INOR.O-2**
Oral Presentation for Young Inorganic Chemists
Room 211+212+213 THU 09:25
Chair: Kyounghoon Lee (Gyeongsang National University)

Fine-Tuning Functional Groups in Metal-Organic Frameworks

Min Kim

Department of Chemistry, Chungbuk National University, Korea

Crystalline, porous, metal-organic frameworks (MOFs) have garnered extensive attention and investigation across various research domains, ranging from fundamental synthesis to practical applications. A distinct advantage of MOFs lies in the remarkable diversity of their structures. These frameworks have been explored with an array of metal clusters and ions, while numerous coordinating ligands have been scrutinized for their synthesis. Moreover, the presence of functional groups on ligand molecules introduces an additional layer of diversity to the core frameworks. The meticulous control of functional groups within MOFs assumes paramount significance in tailoring the desired properties of MOFs for target applications.In this presentation, our recent studies for functional group controls in MOFs will be discussed. Three representative functionalization methods (direct synthesis, PMS: post-synthetic modification, and PSE: post-synthetic exchange) will be introduced. The incorporation of vinyl groups for the synthesis of MOF-polymer composites, the integration of carborane moieties to modulate photophysical properties, and the introduction of tetrazole groups to enhance proton conductivity are expounded. Furthermore, the discussion extends beyond single functional group integration, encompassing dual functionalization schemes along with their ensuing cyclization processes. Noteworthy among these is the positional functionalization of MOFs, where surface modification through ligand exchange has enabled size-selective catalysis, carbon dioxide captures even under humid conditions, and pore functionalization in MOF-polymer composites. Intricate strategies for the installation and application of target functional groups are comprehensively discussed.

Award Lecture in Division : **INOR.O-7**

Oral Presentation for Young Inorganic Chemists

Room 211+212+213 THU 10:30

Chair: Kyounghoon Lee (Gyeongsang National University)

Crystals of Ni_6L_{12} Ellipsoidal Tubes as SCSC Adsorption Matrix: Direct Crystals vs Guest Exchanged Crystals

Ok-Sang Jung

Department of Chemistry, Pusan National University, Korea

The informative difference/similarity between the self-assembled crystals and the SCSC guest exchanged crystals is observed based on both molecular structure and adsorption nature. Self-assembly of $Ni(ClO_4)_2$ with dicyclopentyldi(pyridine-3-yl)silane (L) bidentate in a mixture of toluene and acetonitrile gives rise to purple crystals consisting of double-stranded ellipsoidal tubes, $[Ni_6(ClO_4)_4(CH_3CN)_8L_{12}]8ClO_4{\cdot}4CH_3CN{\cdot}5C_7H_8$. The coordinated acetonitriles as well as solvates of the crystals are removed at 170 °C to transform the purple crystals into the blue crystals of $[Ni(ClO_4)_2L_2]_n$ that return to its original crystals in the mixture of toluene and acetonitrile. Furthermore, toluene and acetonitrile solvates of the original crystals are replaced by o-, m-, and p-xylene isomers within 5 min in a single crystal-to-single crystal (SCSC) manner. The SCSC xylene exchanged crystals are compared with the crystals from the direct self-assembly in the mixture of each xylene isomer and acetonitrile. Self-assembly of $M(ClO_4)_2$ ($M^{2+} = Mn^{2+}$, Co^{2+}, Ni^{2+}, Cu^{2+}, and Zn^{2+}) with dicyclopentyldi(pyridine-3-yl)silane (L) tectonic in the same media, the mixture of acetonitrile and toluene, produces the same crystalline system consisting of M_6L_{12}. The geometry around M^{2+} cations is a typical octahedral arrangement, but their detailed coordination is sensitive to the metal cations depending on subtle ligation competition among perchlorate anion, water, and acetonitrile.

Oral Presentation : **INOR.O-3**
Oral Presentation for Young Inorganic Chemists
Room 211+212+213 THU 09:50
Chair: Kyounghoon Lee (Gyeongsang National University)

Photoproducts Engineering of Metal-Organic Frameworks incorporating Olefin Ligands

Jihye Oh, Jaewook An, In-Hyeok Park[*]

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

In this study, we report photoreactive two-dimensional Zn(II) metal-organic frameworks **1** and **2** with different distances between layers due to each guest molecules. UV irradiation of single crystals of **1** and **2** leads to [2+2] cycloaddition reaction of double bonds in each olefin ligands to produce the cyclobutane rings. Interestingly, through the removal of guest molecules and UV irradiation of **2**, out-of-phase single-dimerized products were obtained between slip-stacked olefin ligands in neighboring layers. Furthermore, by exchanging guest molecules and then UV irradiation of **2**, in-phase single-dimerized products were obtained between parallel aligned olefin ligands within the same layer. Additionally, here we introduce various photo-responsive MOFs incorporating olefin ligands with mono- or di-pyridyl groups.

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

Oral Presentation for Young Inorganic Chemists

Room 211+212+213 THU 10:00

Chair: Kyounghoon Lee (Gyeongsang National University)

Highly Efficient Hydrogen Isotope Separation via Gas(H2)-Liquid(D2) Phase Separation in Mesoporous Media

Jaewoo Park, Hyunchul Oh[1,*]

Chemistry, Ulsan National Institute of Science and Technology, Korea

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

Separating hydrogen isotopes has been a challenging task due to their inherent similarities in size and shape. Currently, cryogenic distillation has been mostly used, but it has a low selectivity of only 1.5 and requires a lot of energy. Alternatively, Quantum sieving technology has been studied mainly on crystalline nanoporous materials such as MOF and zeolite to replace the commercial high-cost separation technology, but it still remains at the fundamental research level.Herein, a new technique for separating isotopes by inducing phase separation of hydrogen is introduced. This can be achieved by creating different liquefaction levels of hydrogen isotopes in the meso pore of a crystalline porous material. This method has the potential to enable isotopic separations at various working conditions (P,T) and larger pores, leading to the development of innovative isotope selection recognition systems. Ultimately, it could make MOF systems suitable for isotope separations.

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

Oral Presentation for Young Inorganic Chemists

Room 211+212+213 THU 10:10

Chair: Kyounghoon Lee (Gyeongsang National University)

Novel Platinum(II) Complexes Based on Tetradentate Ligands and Their High Performances in Blue Phosphorescent Organic Light-Emitting Diodes

Chan Hee Ryu, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Despite the remarkable growth of the organic light-emitting diodes (OLEDs) industry through continuous and extensive efforts to utilize various organometallic luminophores as phosphorescent emitters in the red and green subpixels of OLEDs, blue phosphorescent materials are not practical for OLEDs due to their high emissive energy, which can lead to chemical degradation and decreased efficiency. Therefore, there is a need for improved blue phosphorescent emitters with higher efficiencies and greater electrochemical stability. To meet this need, it is essential to develop an emitter that features a narrow full width at half maximum (FWHM) since this results in greater blue color purity at lower emission energies compared to broad-spectrum emitters, leading to improved stability of the phosphorescent molecules. We herein designed and preparation of a novel tetradentate Pt(II) complexes, Pt3 and Pt4, and their application as blue phosphorescent emitters in OLED devices. The complexes exhibited intense blue emission in the solution and solid states with drastically narrow FWHM (21 nm for Pt3 and 23 nm for Pt4). In addition, these complexes displayed very high phosphorescent quantum efficiencies (93%) with a host materials. Multilayer phosphorescent OLEDs containing Pt3 and Pt4 as emitters with SiCzCz/SiTrzCz2 mixed host systems were fabricated. The devices exhibited outstanding performances, including high external quantum efficiencies (18.6% for Pt3 and 21.0% for Pt4), and operational lifetime (LT_{70} = 3947 h for Pt3 and 1000 h for Pt4 at 200 cd·m^{-2}). These results plainly suggest that this tetradentate Pt(II) dopants are promising candidates as highly efficient, and stable blue phosphorescent emitters in OLEDs.

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

Oral Presentation for Young Inorganic Chemists

Room 211+212+213 THU 10:20

Chair: Kyounghoon Lee (Gyeongsang National University)

New Volatile Strontium Precursors for Next-generation Capacitor in DRAM

Chanwoo Park, Chang Seop Hong[1], Taek-Mo Chung[2,*]

Korea University, Korea

[1]Department of Chemistry, Korea University, Korea

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

Alkaline earth (group 2) metal compounds have numerous uses, including as magnetoresistive materials, ferroelectrics, precursors for thin-film growth, and materials for dynamic random-access memory (DRAM), organic synthesis, and electrically tunable microwave devices. Strontium complexes play a key role in the semiconductor industry because they are used to fabricate thin films containing metal oxides. Among the various ways to deposit thin films, metal-organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) have possibility such as large–area growth, delicate composition control and high film uniformity. Application of alkali metals to these depositions requires highly volatile properties, and our group’s study has focused on design strontium complexes with volatility and stability at high temperature.In this study, we tried the development of strontium complexes using β-diketonate ligands and amino alcohol ligands such as bi- to penta- dentate ligands. When using bi- or tri- dentate ligands, the intermediates strontium complexes are synthesized as dimer and final products were synthesized as trimer complexes, which have low volatility. However, strontium complexes with tetra- or penta- dentate ligands showed high volatility and thermal stability and displayed dimeric structure in final compounds. Especially, most volatile strontium complexes with tetradentate ligand were used to fabricate metal oxide thin film as ALD precursor. All compounds were synthesized via controlled substitution reactions using strontium (II) bis(bis(trimethylsillyl amide)·2DME. Newly synthesized strontium complexes were fully characterized by single crystal XRD analysis, H - NMR, elemental analysis, and thermal gravimetric analysis.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 09:00

Chair: Seung Kyu Min (UNIST)

Electric field-driven molecular memristor and synaptic applications

Chanjin Lim, Junwoo Park*

Department of Chemistry, Sogang University, Korea

Memristor is considered as a promising candidate for the next-generation computing in a sense that memristor enables in-memory processing with a low power consumption. Previous study showed that molecular junctions (BIPY-CoCl2 junctions), based on bipyridine-cobalt complex terminated by alkanethiolates on gold electrode, show both conductance hysteresis and rectification. The hysteric behavior of the molecular junctions depends on the mechanism of the tunneling (i.e. the conductance changes only in the incoherent (Fowler-Nordheim) tunneling regime because the interaction between the hot electrons and the LUMO of the alkyl chain induces the conformational change of the alkyl chain). Here, we demonstrated the modulation of the conductance in the BIPY-CoCl2 junctions with consecutive electric pulses. The pulses in the incoherent tunneling regime increase the conductance (potentiation), while the pulses in the coherent tunneling regime decrease the conductance (depression). The change of conductance varies depending on the amplitude, duration, and interval of the pulse. With the optimized pair of pulses, we were able to observe reversible potentiation/depression cycles. This study shows the possibility of nanometer-sized single-molecule synaptic devices in which the mechanism of the charge transport determines the conductance.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 09:15

Chair: Seung Kyu Min (UNIST)

Interactions of Biologically Active Fluorophores and Graphene Oxide in Neat Solvents and Various Organized Assemblies

Aloke Bapli, Yoonsoo Pang[*]

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

In recent years, introduction of nanotechnology into biological systems has developed new areas of research, such as targeted drug delivery1, biosensing2, bioimaging3, etc. For example, researchers have extensively adopted carbon-based nanomaterials such as graphene, carbon nanotubes, and water-soluble C60, in drug delivery, bio-sensing, gene therapy, and bio-imaging, etc.4-6 These systems may be crucial in understanding various biological processes inside the nanocarrier and also in designing highly effective methods of medical therapy. Among the carbon-based nanocarriers used for the targeted drug delivery, graphene oxide (GO) provides higher bio-compatibility1 and drug-bindings4 due to the presence of oxygen-rich functional groups in the edges and basal planes. Understanding of the fluorophore-nanomaterial interactions would be essential in the potential biological applications of the novel nanomaterials like GO. However, the fluorophore-GO interactions has not extensively been investigated despite the recently growing attentions on the GO in various fields of research. In this work, we have investigated the photophysics of biologically active fluorophores such as Nile Blue A (NBA), Lumichrome, 7-(N, N′-diethylamino)coumarin-3-carboxylic acid (7-DCA) in the presence of GO by steady-state and time-resolved fluorescence spectroscopy. It has been well established that GO generally quenches the fluorescence intensities of fluorophores in many cases including biologically active fluorophore and quantum dots. However, we have found that GO could enhance the fluorescence of some fluorophores depending on the solvent medium. Intrestingly, the photophysical properties of the biologically active fluorophores were significantly modified upon the interaction with GO, both in the absence and presence of various organized assemblies such as serum albumins, reverse micelle, and vesicles. The multifaceted modifications of fluorophore photophysics with GO appear strongly determined by the molecular interactions of fluorophores with GO, and further explorations including other organized assemblies, GO and similar nanostructures are necessary. References:(1) Stobiecka, M.; Dworakowska, B.; Jakiela, S.; Lukasiak, A.;Chalupa, A.; Zembrzycki, K. Sens. Actuators, B. 2016, 235, 136-145.(2) Stobiecka, M.; Chalupa, A. J. Phys. Chem. B. 2015, 119, 13227-13235.(3) Lee, J. H.; Huh, Y. M.; Jun, Y. W.; Seo, J. W.; Jang, J. T.; Song, H.T.; Kim, S.; Cho, E. J.; Yoon, H. G.; Suh, J. S. Nat. Med. 2007, 13, 95-99.(4) Zhang, L.; Xia, J.; Zhao, Q.; Liu, L.; Zhang, Z. Small. 2010, 6, 537-544.(5) Tan, J.M.; Bullo, S.; Fakurazi, S. Sci Rep. 2020, 10, 16941.(6) Sitharaman, B.; Zakharian, T. Y.; Saraf, A.; Misra, P.; Ashcroft, J.;Pan, S.; Pham, Q. P.; Mikos, A. G.; Wilson, L. J.; Engler, D. A. Mol. Pharmaceutics. 2008, 5, 567-578.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 09:30

Chair: Seung Kyu Min (UNIST)

Uncovering Energetic Positions of Surface Trap States in Hematite (α-Fe2O3) Treated with Cobalt Phosphate (Co-Pi) Using Charge Carrier-Selective Heterodyne Transient Grating (CS-HD-TG) Spectroscopic Technique

Young Hyun Kim, Woon Yong Sohn[*]

Department of Chemistry, Chungbuk National University, Korea

Near-field heterodyne transient grating (NF-HD-TG) responses of hematite (a-Fe2O3) treated with cobalt phosphate (Co-Pi) were measured with the burn lasers inducing the depletion of the response by the removal of the trapped charge carriers in the target state, which is called charge carrier-selective heterodyne transient grating (CS-HD-TG) spectroscopic technique. We found that two distinct trap states co-existed in Co-Pi loaded on the surface of a-Fe2O3. One of them named r-SS2, of which potential was similar to that of r-SS1 in the surface of a-Fe2O3, acted as a recombination centre but could increase the lifetime of the trapped holes by the charge separation, consistent with the previous study. We also revealed that the energetic position of the other (i-SS2), which has been regarded as the intermediate state for oxygen evolution reaction with low overpotential, was higher than that of i-SS1 in a-Fe2O3 but lower than those of r-SS1 and r-SS2.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 09:45

Chair: Seung Kyu Min (UNIST)

Photochemical Dynamics of V-PYRRO/NO Investigated by Time-resolved IR Spectroscopy

Hojeong Yoon, Manho Lim*, Seongchul Park, Seong Beom Jeon

Department of Chemistry, Pusan National University, Korea

In this study, we investigated a novel compound, O(2)-vinyl 1-(pyrrolidin-1-yl)diazen-1-ium-1,2-diolate (V-PYRRO/NO), with potential applications in selective NO release within the liver. This compound possesses the ability to release nitric oxide (NO) at low concentrations, inducing vasodilation, and at high concentrations, triggering apoptosis in cancer cells. It is enzymatically converted within the liver to diazeniumdiolate (NONOate). Our focus was to unravel the mechanism of NO release from V-PYRRO/NO using light-based approaches.Initially, we employed femtosecond laser-driven time-resolved IR spectroscopy (TRIR) to study V-PYRRO/NO dynamics excited by 300 nm photons, designed to induce π-π^* transitions of NO. Combining quantum chemical calculations and molecular dynamics simulations, we predicted the photochemical reaction mechanism. Consequently, upon irradiation at 300 nm, V-PYRRO/NO dissociated into forms where NO bound to pyrrolidine resulted in N-nitrosopyrrolidine and ethenyloxynitrene (vinyl-ON) species. This interpretation was substantiated by rationalizing the observed dynamics through the potential energy surface (PES) obtained from CASSCF calculations.Furthermore, in order to elucidate the transformation of the vinyl-ON species in different solvents, we analyzed peak shifts through experiments involving methanol-d4 and acetonitrile-d3. The shifts were attributed to D^+ (deuterium cation)-mediated changes and reveal the chemistry of vinyl-ON.The results of this study have contributed to understanding the light-induced chemical dynamics of V-PYRRO/NO molecules, and future studies are planned to improve the NO release mechanism and seek new application possibilities by investigating the reaction under higher energy conditions.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 10:00

Chair: Seung Kyu Min (UNIST)

Crystallization of Amorphous Solid Water Affected by Porosity Control

Du Hyeong Lee

Korea Polar Research Institute, Korea

Amorphous solid water (ASW) is a metastable phase of water that exists at cryogenic temperatures below ~130 K, and transforms into crystalline ice as temperature rise. This study investigates the effect of deposition temperature of ASW on its crystallization behavior. The experiments were conducted using thin ASW films deposited by backfilling water vapor onto a Pt(111) crystal under ultrahigh vacuum condition. Porous ASW prepared at 90 K predominantly exhibited bulk-initiated crystallization, whereas ASW prepared at 125 K exhibited surface-initiated crystallization. The results suggest that nucleation in bulk can occur in porous ASW, but it is suppressed in nonporous ASW prepared at high temperatures. These findings offer valuable insights into water's behavior in low-temperature environments, such as the interstellar medium.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 10:15

Chair: Seung Kyu Min (UNIST)

A Novel Dataset and Model for Organic Reaction Mechanism Prediction

Joonyoung F. Joung, Connor W. Coley*

Department of Chemical Engineering, Massachusetts Institute of Technology, United States

Predicting organic reaction outcomes is crucial in various fields, like drug discovery and materials science. Understanding reaction mechanisms enables precise control of reactions and optimizing conditions. While machine learning models can predict reaction outcomes based on given reactants, explaining the reaction mechanisms remains a significant challenge. Despite the abundance of organic reaction datasets containing reactant-product pairs, the lack of mechanistic datasets hinders the potential of machine learning models to explain the mechanisms behind these predictions.In this talk, we present a novel dataset of organic reaction mechanisms, containing over 5 million elementary reactions. This dataset was constructed by applying expert mechanistic templates of 100 reaction types to a collection of 4.4 million unique reactions extracted from US and European patents from 1976 to the present. Utilizing this dataset, we trained a graph neural network capable of predicting intermediate species formed during reactions.We evaluated the model's accuracy in predicting the next intermediate species and reaction outcomes through multiple elementary reaction steps. Additionally, our model can identify critical steps leading to impurity formation, particularly important for pharmaceutical industries. Furthermore, its generalizability was demonstrated by accurately predicting reaction outcomes for previously unseen reaction types.Our findings bridge the gap between predicting reaction outcomes and mechanistic understanding. The insights gained from our study not only advance our understanding of organic reactions but also pave the way for enhanced control over these reactions, offering opportunities for optimizing chemical processes.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 10:30

Chair: Seung Kyu Min (UNIST)

A Machine Learning Strategy for a Hidden Structural Origin of Two-Dimensional Colloidal Glass Transition

Eun Cheol Kim, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Glassy environments can be observed in various systems, but the underlying structural origin of their glassy dynamics is still unknown. Because the glass states and the liquid states have similar structures, it is hard to distinguish glasses from liquids solely based on structural information. We construct convolutional neural network (CNN) machine learning models to find a hidden origin of glass transition based on the structures. We introduce two kinds of glassy systems: a two-dimensional polydisperse colloidal system (PC) and a two-dimensional binary colloidal system (BC). These systems can be an excellent test bed for finding structural information of glass transition because PC glasses have a large hexatic medium-range crystalline order (MRCO), but BC glasses do not. Our CNN models successfully distinguish images of glass configuration from liquid configuration. This implies that the states of the colloidal system can be classified accurately only with structural information. Furthermore, the CNN models trained with BC glasses and liquids (without hexatic MRCO in glass states) can predict the states of PC glasses and liquids (with a large hexatic MRCO in glass states), thus indicating that the hexatic MRCO should not be the critical structural information of glass transition and there could be more general structural origin of glass transition in the region where the CNN models assign weights.

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

Oral Presentation for Young Physical Chemist

Room 208+209+210 THU 10:45

Chair: Seung Kyu Min (UNIST)

Density-Corrected DFT for Large Molecular Systems

Mingyu Sim, Eunji Sim*, Youngsam Kim

Department of Chemistry, Yonsei University, Korea

Kohn-Sham Density Functional Theory (KS-DFT) is a popular method for electronic structures calculations due to its optimal balance between accuracy and computational cost. In many conventional DFT calculations, the self-consistent densities approximate the exact densities well, but there are some exceptions. Recently, HF-r2SCAN-DC4, grounded in density-corrected DFT (DC-DFT) principles, has shown that replacing the self-consistent densities with Hartree-Fock (HF) densities, complemented by dispersion corrections (DC4), can notably reduce DFT energy errors. However, computing HF densities using large basis sets for large molecular systems is highly cost-prohibitive. In this study, we show that the accuracy of HF-r2SCAN-DC4 for small molecular systems is consistently maintained even when applied to large molecular systems. Also, we demonstrate that for large molecular systems, using the dual-basis method to obtain HF density allows DC-DFT to achieve accurate results with significantly reduced computational demands.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:00

Chair: Sungju Yu (Ajou University)

Investigating Surface Plasmon Damping and Fano Resonance Induced by Epitaxial Growth of Palladium on Single Gold Nanorods

Metya Indah Firmanti, **Ji Won Ha**[1,*]

Chemistry, University of Ulsan, Korea

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

Plasmon damping and Fano resonance induced in the growth of palladium (Pd) on gold nanorods (AuNRs) are poorly understood. Herein, we investigated the optical properties of single AuNRs@Pd (core@shell) synthesized using epitaxial Pd growth at different Pd concentrations. Core@shell AuNR@Pd demonstrated metal-induced surface damping, as evidenced by the red-shift and linewidth broadening. Addition of thiols to the bimetallic nanoparticle system revealed the competition between metal and chemical surface plasmon damping, as indicated by the real-time results of benzenethiol chemisorption involving various groups. The localized surface plasmon resonance (LSPR) spectra of single AuNRs@Pd on higher Pd concentrations showed characteristic subradiant and superradiant peaks, as well as Fano resonance as a spectral dip, which was highly influenced by the Pd shell thickness. The occurrence of Fano resonance during the Pd growth was further verified by in situ real-time observation experiments. We then elucidated time-dependent, real-time variations in LSPR peak wavelength, metal-induced surface damping, and Fano resonance mode of single AuNRs@Pd. Therefore, this study provides new insights into metal interface damping, the Fano resonance, and optical tunability by engineering Fano resonance energy and Pd shell thickness.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:04

Chair: Sungju Yu (Ajou University)

Localized Surface Plasmon Decay Pathways competition on Mesoporous Silica Coated Gold Nanorods Amalgamation

Yola Yolanda Alizar, Ji Won Ha[1,*]

Chemistry, University of Ulsan, Indonesia

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

This study aims to investigate the effects of mercury (Hg)-induced amalgamation and thiolation on mesoporous silica-coated gold nanorods (AuNRs@mSiO_2) by looking at LSPR single spectra and FWHM changes using Dark-Field (DF) Microscopy and Spectroscopy. First, the morphology of AuNRs@mSiO_2 exposed to Hg solution and 1-alkanethiol solution did not change due to the silica shell that prevented the AuNR core from deformation. Secondly, DF microscopy and spectroscopy observed a blue shift of the LSPR energy wavelength and plasma damping in the scattering spectra of AuNRs@mSiO_2 single particles exposed to Hg solution. Interestingly, a red shift is shown in the LSPR and a narrowing of the line width due to the strong interaction between Hg and the -SH functional group of the thiol and making a complex reaction. In comparison with expanding Hg exposed on a single AuNR@mSiO_2, the LSPR is red-shifted due to slow inward diffusion and narrowing of the FWHM. When the substrate is changed to thiol, the LSPR shows more red shift due to the strong intensity surface of the Au-Hg core shell interacting with -SH. Finally, compared to Hg exposed to the same amount of thiol carbon, the FWHM has a strong attenuation due to Au-Hg that has become an alloy that allows Au to interact with thiols. Therefore, this work presents a new strategy to study to detect Hg incorporation using the LSPR energy wavelength of AuNRs@mSiO_2 single particles and study the interfacial attenuation by looking at the interaction between Au, Hg, and -SH groups.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:08

Chair: Sungju Yu (Ajou University)

Defining Co-resistance Mechanisms in Cytarabine-resistant Human Acute Myeloid Leukemia Cells Using Biochemical Analysis

Jinhui Kim, Sooyeon Chae

Department of Chemistry, Korea University, Korea

Acute myeloid leukemia (AML), which accounts for more than 80% of adult cases of leukemia, is a blood cancer that spreads quickly and starts in the bone marrow. For the past 40 years, combination of cytarabine (ARA-C) and daunorubicin (DNR) has been widely used as an AML treatment regimen. However, only 40% of patients who receive the ARA-C/DNR regimen achieved complete remission, and 60% of patients experience AML relapse after standard treatment. Even though there have been several studies on the mechanism of resistance to the two anticancer drugs, there hasn’t been enough done on the common resistance to this two-drug regimen. We investigated the co-resistance of ARA-C and DNR in this work with the goal of elucidating this phenomenon through biochemical study. The normal AML cell line SHI-1 and the cytarabine-resistant cell line R640-SHI-1 were both treated with ARA-C and DNR separately or simultaneously, and cell viability was then measured. As a result of data analysis, It was confirmed that the R640-SHI-1 developed DNR resistance. These finding led us to assume that the R640-SHI-1 cell line not only exhibited ARA-C-specific resistance mechanisms but also a general resistance mechanism that contributed to both ARA-C and DNR resistance. To determine whether drug resistance is related to the amount of drug uptake by cells, we will measure the amount of cellular drug uptake by various analytical methods. Moreover, the co-resistance mechanism will be traced through proteomic analysis of cells, and analysis of micro-RNA components in exosomes.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:12

Chair: Sungju Yu (Ajou University)

Gas chromatography and Paper spray ionization mass spectrometry for the analysis and differentiation of eucalyptus oils

Heejin Ro

Chemistry, Dongguk University, Korea

Eucalyptus oils have been widely used in various household chemical products including mouthwash, insect repellents, and ointments. There are more than 300 species of eucalyptus, and the commonly used types are Eucalyptus(E.) globulus, E. citriodora, and Australian types. Each of these species is listed by the International Organization for Standardization (ISO) with data on its composition and content. Chemical analysis of eucalyptus oil is typically performed by gas chromatography (GC) with mass spectrometry (MS) for qualitative analysis and flame ionization detection (FID) for quantitative analysis. In this study, we developed a method to analyze eucalyptus oil by paper spray ionization MS (PSI-MS) to find its chemical fingerprint quickly and effectively. With PSI, it can be analyzed quickly under atmospheric pressure and even with a small amount of samples. For the detection of characteristic components of eucalyptus oil, including eucalyptol and citronellal, we optimized the parameters for PSI, including spray solvent composition, spraying voltage, and paper substrate. GC-MS, GC-FID, and optimized PSI-MS were used to obtain chemical fingerprints that could distinguish the species of three different eucalyptus oils. Then, chemical fingerprint data obtained from three different analytical platforms were subjected to principal component analysis (PCA) for type-difference performance evaluation. These studies demonstrate that GC-MS, GC-FID and PSI-MS data combined with PCA could be used to determine the type of unknown eucalyptus oil and also to examine their mixing ratios.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:16

Chair: Sungju Yu (Ajou University)

Volatile organic compounds (VOCs) capture with Deep eutectic solvents (DESs) and analysis by headspace gas chromatography mass spectrometry

Seo Young Hwang

chemistry, Dongguk University, Korea

Volatile organic compounds (VOCs), one of the substances we come into contact with the most in our daily lives, are one of the main components of air pollutants. Some VOCs have harmful effects on the human body and can cause various diseases. Therefore, it is necessary to captuere these VOCs. Absorbents that have been tested for VOCs include aqueous solutions, silicone oils, adipates, and ionic liquids. However, these absorbents are limited by poor capture efficiency, high cost, and toxicity. To address these shortcomings, green solvents called deep eutectic solvents (DESs) are emerging as a new class of absorbents for airborne VOCs. Unlike previously used solvents, DESs have the advantages of being inexpensive, easy to make, non-toxic, and have good VOC absorption efficiency. In this study, we tested the VOC absorption efficiency of various DESs and compared the performances of tested DESs to those of conventional VOC absorbents. We also developed a method for analyzing the VOCs captured in DESs using headspace-gas chromatography mass spectrometry (HS-GC-MS). DESs generally showed higher stability and capture efficiency of VOCs than conventional absorbents and thus allowed sensitive detection of trace VOCs.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:20

Chair: Sungju Yu (Ajou University)

Improving accuracy for determination of active pharmaceutical ingredient concentration in tablets with varying compaction density using oversampling strategy

Haeseong Jeong, Hoeil Chung[*]

Department of Chemistry, Hanyang University, Korea

In pharmaceutical tableting process, depending on the applied compaction force, certain components may undergo physical/chemical alterations which affect their crystal structure or particle size in sequence. Therefore, these subtle changes alter the spectral features of tablets and thereby hinder the precise quantitative spectroscopic measurements. To overcome the potential degradation of accuracy under the variation of compaction density, oversampling algorithm was proposed. It was to generate multiple spectra of tablets potentially reflecting the change of compaction density in prior and use them to build a compaction density-tolerant prediction model using partial least squares (PLS). For this study, the tablets containing paracetamol as an active pharmaceutical ingredient (API) (concentration: 3 - 21%, increments of 2%) prepared with three different pressures (40, 60, and 80 kgf/cm2) were employed. Near-infrared (NIR) and Raman spectra of the tablets were collected, and these acquired spectra were combined with the spectra generated with using oversampling algorithm for the determination of API concentrations using PLS. The accuracies with and without using oversampling algorithm were mutually compared and utility of oversampling algorithm was discussed.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:24

Chair: Sungju Yu (Ajou University)

[Withdrawal] Characterization of pore-forming Amyloid Beta Protein using NMR Spectroscopy

Joohan An, Yongae Kim*, Minseon Kim

Department of Chemistry, Hankuk University of Foreign Studies, Korea

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Oral Presentation : **ANAL1.O-8**
Oral Presentation of Young Analytical Chemists
Room 214 THU 09:28
Chair: Sungju Yu (Ajou University)

[Withdrawal] A hybrid carbon/solid-electrolyte coating on Fe3BO5 conversion type anodes for ultra high C-rate applications

Rajeev Kumar, **Dung Nguyen**[1], **Jeongin Kim**[2], **Youngil Lee**[3,*]

Chemical Industry Research Institute, University of Ulsan, Korea
[1] *Chemical Industry Research Institution, University of Ulsan, Korea*
[2] *University of Ulsan, Korea*
[3] *Department of Chemistry, University of Ulsan, Korea*

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:32

Chair: Sungju Yu (Ajou University)

SABRE Hyperpolarization of Nicotinamide Derivatives and its Chemical Kinetic Properties

Quy Son Luu, Thi Quynh Nguyen[1], SeokKi Yun[2], Jae Hwa Choi[2], Youngbok Lee[3,*]

Bionanotechnology, Hanyang University, Korea
[1]*Department of Applied Chemistry, Department of Bionano Convergence , Korea*
[2]*Applied Chemistry, Hanyang University, Korea*
[3]*Department of Bio-Nano Engineering, Department of, Korea*

Nicotinamide derivatives play an essential role in biomedicine, such as the nicotinamide adenine dinucleotide (NAD+), which is an electron carrier in the glycolysis and citric acid cycle (known as the Krebs cycle). In addition, they are also commonly used in the production of dietary supplements (such as vitamin B3), which help us improve the appearance of fine lines, wrinkles, hyperpigmentation, and acne. Understanding the metabolism and pharmacological effects of nicotinamide derivatives is important in pharmacology. This knowledge helps in designing drug regimens and evaluating drug interactions. Hence, we utilized SABRE (signal amplification by reversible exchange) hyperpolarization using a home-built system to study the details of the pharmacokinetics of nicotinamide derivatives. This method helps us overcome the main limitation of conventional NMR (nuclear magnetic resonance), such as its low sensitivity. To prove the concept, we hyperpolarized benzyl nicotinamide (BnNCA) and nicotinic acid hydrazide (NTH). We investigated the effect of magnetic field, bubbling time, and co-ligand on the hyperpolarized efficiency of these compounds. Alongside, T1 relaxation time with and without iridium catalyst (a spin order transfer catalyst in the SABRE technique) was determined by using inversion recovery and a single shot at a small flip angle or manual method at thermal and hyperpolarization conditions, respectively. For example, the 1H NMR of BnNCA with DMSO-d6 as a co-ligand exhibited the highest enhancement factor ($\varepsilon H2 = 103$) at 6.5 mT, 90 s, and 3 atm of 50% para-hydrogen and the T1

relaxation time of proton (H2) in BnNCA and NTH at hyperpolarized is 16 s and 9 s, respectively. This long T1 relaxation time is helpful in the studying organic reaction monitoring.

Oral Presentation : **ANAL1.O-10**
Oral Presentation of Young Analytical Chemists
Room 214 THU 09:36
Chair: Sungju Yu (Ajou University)

CRISPR/Cas13a-mediated SERS-based dual-flow assay strips for amplification-free detection of SARS-CoV-2 RNA

Younju Joung, Soyeon Lee, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

The gold standard method for diagnosing SARS-CoV-2 target gene is RT-PCR. However, amplifying the target gene requires a 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 first channel, followed by the sequential flow of SERS nanotag solution through the second channel. This sequential flow arrangement allows for both CRISPR/Cas reaction and 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-11**

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:40

Chair: Sungju Yu (Ajou University)

Investigation of Light-Responsive Microcapsules Based on Renewable Materials

Uyen Thi Do, Quy Son Luu, Seyoung Yang[1], Minji Song[1], Youngbok Lee[2,*]

Center for Bionano Intelligence Education and Research, Hanyang University, Korea
[1]*Hanyang University, Korea*
[2]*Department of Bio-Nano Engineering, Department of, Korea*

The escalating environmental impact of petrochemical plastics and their persistence in the environment has spurred the quest for biodegradable alternatives sourced from renewable materials. A promising contender in this regard is polylactic acid (PLA), distinguished by its biorenewable, biocompatible, and biodegradable attributes. This study investigates into innovatively incorporating azobenzene (AZO) into PLA matrices, giving rise to light-responsive PLA composites. Furthermore, a precipitation method was employed to subsequently fabricate microcapsules with on-off light-switching capabilities. Employing 1H and 13C-NMR, we probed the structural intricacies of both conventional PLA and AZO-PLA. Results reveal the successful synthesis of low-molecular-weight (L)-PLA from lactic acid monomers and confirm the integration of light-responsive AZO moieties into PLA chain, as evidenced by distinctive aromatic signals in the NMR spectra of AZO-PLA. Intriguingly, reversible photoisomerization was achieved via alternating irradiations at 365 nm and 450 nm with no apparent fatigue phenomenon, as evidenced by UV-Vis results, indicating that AZO-PLA presents good light-convertibility. Furthermore, the study characterizes microcapsules based on AZO-PLA through microscopy and NMR analyses. These findings highlight the successful generation of small spherical capsules, thus expanding the potential applications of the synthesized polymers. Looking forward, our research will elucidate the light-responsive mechanisms triggering the release of AZO-PLA-based microcapsules and explore the potential reusability of the synthesized capsules.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:45

Chair: Sungju Yu (Ajou University)

A Comprehensive Study of Conformational Changes in Malachite Green Using Electrochemistry-SERS

Wiyogo Prio Wicaksono, Jaeuk Ahn, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

The pH-sensitive and electroactive characteristics of malachite green (MG), a cationic dye, potentially affect the spectra of surface-enhanced Raman spectroscopy (SERS) in electrochemical SERS (EC-SERS) analysis. This study presents a comprehensive EC-SERS investigation to obtain dynamic SERS spectra of MG on Au SERS substrates at various applied potentials. Initially, cyclic voltammetry (CV) was performed on MG to determine an appropriate EC-SERS potential window, the mass and electron transfer mode involved in the redox process, and the number of electrons and protons participating. Furthermore, various parameters of EC-SERS were optimized, including pH and the type of supporting electrolytes. The results indicate that the highest SERS signal can be achieved through chronoamperometry SERS (CA-SERS) and CV-SERS at an applied potential of 0.6 V (vs. Ag/AgCl) using 0.1 M phosphate buffer at pH 4 as the supporting electrolyte. Plausible mechanisms for electrooxidation and the enhancement of the SERS signal were proposed. Interestingly, the oxidized form of MG, its conformational changes, and the transformation of adsorption orientation were successfully elucidated through CV-SERS. Finally, this work provides molecular-level insights into the adsorption orientation of MG and its oxidized form. This involves aromatic rings with a tilted upright orientation at positive applied potentials. These findings confirm a clear understanding of the enhancement mechanism of the SERS signal, which is valuable for developing EC-SERS-based MG sensing.

Oral Presentation : **ANAL1.O-13**
Oral Presentation of Young Analytical Chemists
Room 214 THU 09:50
Chair: Sungju Yu (Ajou University)

Radical and 29Si-isotope enrichment silica nanoparticles for 29Si Dynamic Nuclear Polarization

Thi Quynh Nguyen, Seyoung Yang, Minji Song, Youngbok Lee[1,*]

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

Silica nanoparticles possess favorable characteristics for their potential use as a promising 29Si MRI probe. To fully harness the capabilities of silica material in MRI applications, the Dynamic Nuclear Polarization (DNP) technique can be effectively employed to significantly amplify NMR signals. In the present investigation, silica nanoparticles were selectively embedded with a uniform global concentration, along with a consistent 29Si-isotope ratio. These nanoparticles were strategically modified in different regions: encompassing the entire particle structure, focusing solely on the first/second 10 nm shell, or the 20 nm shell in unique onion-like configurations (core@shell@shell particles). The presence of TEMPO radicals within these particles was confirmed through EPR measurements, while the quantification of 29Si nuclei in each sample was validated using solid-state NMR techniques. These specialized particles exhibit the potential for self-polarization in DNP, and their hyperpolarization will be further investigated. This study aims to elucidate an efficient strategy for enriching both 29Si isotopes and radicals, paving the way for the advancement of 29Si MRI probe development.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 09:55

Chair: Sungju Yu (Ajou University)

Comparison of the performance of thickness-tapered channel in flow field-flow fractionation with the effect of field programming in a uniform channel

Jaihoo Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Flow field-flow fractionation (flow FFF) is a elution-based method to separate particulate materials by size. In flow FFF, carrier liquid flows along the thin rectangular channel space, with crossflow acting across the channel as a driving force of separtion. Field programming in flow FFF is achieved by varying crossflow rate with time and it is efficient to elute long retaining materials in a fast time without losing resolution. However, it typically requires a special flow rate controller.Thickness-tapered channel in flow FFF was recently introduced by decreasing the channel thickness along the channel in order to increase the separation speed without using field programming and to improve separation efficiency and recovery without an expensive flow controller. In this study, the particle separation with field programming in flow FFF of uniform thickness channel is compared with the thickness-tapered channel without field programming in terms of separation efficiency and speed.

Oral Presentation : **ANAL1.O-15**
Oral Presentation of Young Analytical Chemists
Room 214 THU 10:00
Chair: Sungju Yu (Ajou University)

Lipid perturbation in brain and spleen tissues of mice caused by SARS-CoV-2 using nanoflow UHPLC-ESI-MS/MS

Hwangyu Park, Myeong Hee Moon[1,*]

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

In the 21st century, in addition to SARS-CoV-2, various other corona virus diseases such as SARS and MERS were prevalent. Due to the characteristics of continuous mutation and zoonotic infection, it is expected to remain a concern in the future. That is why the need for research is emerging because the betacoronavirus genus shows similar patterns in symptoms, infection, and metabolic pathways. Lipids play a critical role in viral entry, replication, and assembly and involve in many pathological symptoms. Therefore, lipidomic research data accumulation can aid in early diagnosis and treatment strategies. To assess how SARS-CoV-2 affects the spleen and brain tissues based on varying virus injection doses and the days post-infection, the study conducted both qualitative and quantitative lipidomic analysis at six different time points using mice infected with two different levels of plaque-forming units (PFU), comparing them to a control group. In this study, we investigated the lipid profiles of the spleen and brain tissues of SARS-CoV-2-infected mice using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry. The non-targeted comprehensive analysis identified a total of 593 and 926 lipids in the brain and spleen tissue. Notably, targeted quantification revealed significant alterations in the majority of lipids within the infected group, regardless of the infection dosage.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:05

Chair: Sungju Yu (Ajou University)

Biomarker discovery in prostate cancer from 20 cancer patients with tissue proteomics

Junghoon Kang, Miseon Jeong, Yunseon Woo, Seung Jeong Lim, Wonryeon Cho[*]

Department of Chemistry, Wonkwang University, Korea

The early diagnosis of prostate cancer (PCa) is based on digital rectal examination (DRE) and/or serum prostate-specific antigen (PSA) level. However, these tests are neither sensitive nor specific enough to detect clinically significant PCa leading to overdiagnosis, such as unnecessary biopsies. This study intended to discover PCa-specific biomarker candidates from PCa tissues with shotgun proteomics for a more accurate early diagnosis.Twenty PCa tissues were collected from PCa patients with different PSA levels in blood test. The each PCa tissue was homogenized individually, and proteins were extracted using lysis buffer without detergent from the homogenized PCa tissues. Then the supernatant fluid was trypsin digested and desalted respectively, and the proteomes in each PCa tissue were identified and quantified with multiple nLC-MS/MS analyses and protein database search software. Proteomes in each PCa tissue were comparatively analyzed according to the clinical information of PCa patients, and proteins found commonly in 20 PCa tissues were identified.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:10

Chair: Sungju Yu (Ajou University)

Characterization of serum exosome lipids from patients with cholangiocarcinoma by nUHPLC and mFIFFF coupled with ESI-MS/MS

Hyeju Yu, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Cholangiocarcinoma carries a very poor prognosis. There are two types of cholangiocarcinoma, intrahepatic and extrahepatic. Each type has a different treatment method, so a differential diagnosis is required. Therefore, it is desired to identify potential biomarkers capable of distinguishing and diagnosing the two cholangiocarcinomas. Exosomal lipids, which are closely related to intercellular communication and have a limited size, can be useful biomarkers for lipid-related diseases.This study aims to demonstrate the potential of top-down analysis of mFIFFF-ESI-MS/MS as a high-speed screening platform by comparing the results of bottom-up analysis. Exosome lipids were analyzed through bottom-up analysis by nanoflow ultrahigh performance liquid chromatography-tandem mass spectrometry (nUHPLC-ESI-MS/MS) and top-down analysis by miniaturized asymmetrical flow field-flow fractionation and electrospray ionization-tandem mass spectrometry (mFlFFF-ESI MS/MS).Exosomes were isolated from serum samples of patients diagnosed with intrahepatic cholangiocarcinoma (ICC, n=15), extrahepatic cholangiocarcinoma (ECC, n=15), and control (C, n=15) using ultrafiltration. As a result of lipid analysis using nUHPLC-ESI-MS/MS, 966 lipids were identified, 291 lipids were quantified, and 61 lipids showing a 1.5-fold difference were selected as potential biomarker candidates. A top-down analysis will be performed on these selected targets. The Top-down analysis has been optimized to be completed in approximately 10 minutes and confirmed exosomal lipid detection.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:15

Chair: Sungju Yu (Ajou University)

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

Ji Yeong Lee, Hwangyu Park[1], Myeong Hee Moon[2,*]

Chemistry, Yonsei University, Korea

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

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

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 processes result in changes in lipid composition. In this study, the recovery process from the infection 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 and 869 lipids were identified in the lung and liver samples from mice through qualitative analysis. At 1x102 PFU (plaque forming unit), most lipid classes exhibited substantial decreases in lung tissue at 2 days post-infection (dpi), followed by subsequent recovery. Similarly, at 1x105 PFU, 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. 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 : **ANAL1.O-19**
Oral Presentation of Young Analytical Chemists
Room 214 THU 10:20
Chair: Sungju Yu (Ajou University)

Optimization of skin sampling method for lipidomic analysis via nanoflow nUHPLC-ESI-MS/MS

Seunghee Shin, Myeong Hee Moon[1,*]

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

Human skin functions as a primary physical barrier against the external environment. The primary components of the outermost epidermal layer, known as the stratum corneum, consist of lipids like ceramides and glycerolipids. To efficiently sample the skin, tape stripping is commonly used, where an adhesive tape is used to collect the stratum corneum layers. Since there are several variables that affect the amount of lipids removed by each tape strip, a standardized sampling procedure is required. This study aimed to optimize skin sampling method in terms of sampling location and the number of tape strips in case of repeated stripping. Skin samples were collected from ten consecutive tape strips at the same spot, as well as from five successive tape strips at four different locations (forehead, forearm, cheek, and neck). were taken and their lipids were analyzed 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, alongside minor changes in lipid composition. This decrease became significant after the 6th strip.To overcome the strip to strip variation in lipid composition, a pooling method of different strips was adopted. Extracts from the first 3 or 5 consecutive tape strips were pooled, respectively, and analyzed. This approach resulted in the identification of over 100 additional lipid species in the pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strip 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 : **ANAL1.O-20**

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:25

Chair: Sungju Yu (Ajou University)

Raman spectroscopic quantification of microplastic particles in water using polydimethylsiloxane-coated nickel foam as a particle-capturing platform

Sangjae Kim, Hoeil Chung[*]

Department of Chemistry, Hanyang University, Korea

Nickel foam (NF) was utilized as a microplastic particle-capturing medium in this study. NF is hydrophobic and porous, it could attract microplastic particles such as polyethylene (PE) particles and hold them inside. Nonetheless, the average recovery was 69.5% and unsatisfactory when the NF was used to capture PE particles in water samples. To increase the hydrophobicity, a circular polydimethylsiloxane (PDMS)-coated NF (PDMS-NF, diameter: 6 mm) was prepared and tested. The resulting recovery was elevated to 97.6% owing to the increased hydrophobicity of PDMS-NF confirmed by a contact angle measurement. Next, to quantify the PE particles captured by the PDMS-NF using Raman spectroscopy, a wide area illumination (WAI) scheme providing a laser illumination diameter of 6 mm was adopted to fully cover the PDMS-NF. The intensity ratios of PE and PDMS peaks in the collected spectra linearly increased with the quantities of dispersed PE particles (0.1~4.0 mg range, R2: 0.992) in water samples.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:30

Chair: Sungju Yu (Ajou University)

LC-MS based metabolomic analysis of plasma from a severe COVID-19 patient treated with ECMO

Yourim Shin, **Youngae Jung**, **Geum-Sook Hwang**[1,*]

Western Seoul Center, Korea Basic Science Institute, Korea

[1]*Korea Basic Science Institute, Korea*

Coronavirus disease (COVID-19) is a respiratory infection that can cause severe respiratory symptoms in some patients. In the case of severe patients, a treatment method called Extracorporeal Membrane Oxygenation (ECMO) can be considered because the oxygen supply is insufficient due to inflammation and damage to the lungs. In this study, we observed changes in plasma metabolites between individuals who survived and those who deceased following ECMO treatment using liquid chromatography tandem mass spectrometry (LC/MSMS).We collected plasma samples from 31 COVID-19 patients who received ECMO treatment between 2021 and 2022. Among these, there were total 84 plasma samples, including 52 samples from surviving group and 32 samples from deceased group, obtained at four different longitudinal time points.Partial least squares-discriminant analysis (PLS-DA) score plot generated from 60 quantified metabolites showed a separation between surviving group and deceased group. Importantly, using initial plasma samples, we observed significant changes in six metabolites between the surviving and deceased groups. Cystathionine, asparagine, arginine, phenylalanine, pyridoxine, and urea showed a decreasing trend as plasma collection rounds were progressed in surviving group. In contrast, these metabolites except for asparagine exhibited a slight increase in the deceased group.This study demonstrates that metabolomic analysis using LC/MSMS is useful for observing the plasma metabolites of deceased and surviving patients after ECMO treatment.

Oral Presentation : **ANAL1.O-22**
Oral Presentation of Young Analytical Chemists
Room 214 THU 10:35
Chair: Sungju Yu (Ajou University)

Untargeted Metabolomic Analysis of Liver Tissues for Mouse Infected with Covid-19

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

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

At the end of 2019, SARS-CoV-2 emerged and caused a global pandemic characterized by severe pneumonia, multi-organ failure, and death. Several studies have reported cases of acute liver damage and liver failure in response to coronavirus infection, but the hepatic metabolic changes caused by SARS-CoV-2 have not been clearly identified. This study will provide insight into metabolic pathways involved in liver dysfunction in SARS-CoV-2 infection. We obtained liver tissue samples from hACE2 mice intranasally infected with 10^2 wuhan virus at 2 dpi, 5 dpi, 7 dpi, 14 dpi and control (no infection). Analysis of liver tissue from SARS-CoV-2 infected mice was performed by untargeted metabolomics approach using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS). The Principal Component Analysis (PCA) score plots, a supervised multivariate data analysis method, was conducted to examine differences according to dpi in both the positive and negative ion mode. And then, kruskal-wallis test was performed and a total of 75 metabolites showed significant changes after infection with SARS-CoV-2. K-Means Clustering was performed to confirm the tendency, and it was possible to confirm the pattern of increasing after 7 day, decreasing pattern after 7 day, and increasing pattern from 2 day to 14 day. Through these pattern changes, it can be confirmed that various metabolic changes occur in the liver after infection. The results of this study suggest that LC/MS-based untargeted metabolomics can be a useful tool for understanding hepatic metabolic changes caused by SARS-CoV-2 infection.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:39

Chair: Sungju Yu (Ajou University)

LC-MS-based lipidomics reveals disrupted lipid metabolism in macrophages exposed to particulate matter

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

Western Seoul Center, Korea Basic Science Institute, Korea

[1]*Korea Basic Science Institute, Korea*

Particulate matter (PM) is a major environmental concern worldwide and has been reported to cause health problems including diabetes and atherosclerosis. Emerging evidence suggests that macrophages, as innate immune cells, play a key role in regulating lipid metabolism within biological systems. However, studies on the underlying molecular mechanisms linking PM exposure and its impact on cellular responses such as lipid metabolism and inflammation are poorly understood. In this study, we investigated PM-induced lipidomic changes and their associations with inflammation in macrophages. Raw 264.7 macrophage cells were exposed to PM10-like fine dusts (CZ100) and PBS (control group). Then, the extracted lipidome of macrophage cells was profiled using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry. As a result of multivariate analysis, the principle component analysis score plots showed clear separations between CZ100 and PBS groups. And, we observed significant alterations in the lipidomic profiles of macrophatges exposed to PM. Specifically, the levels of lysophosphatidylcholines, lysophosphatidylethanolamines, ceramides and very-long chain fatty acids were remarkably increased in CZ100 cells compared to PBS cells, whereas those of plasmanyl-phosphatidylethanolamines and phosphatidylinositols were significantly decreased in CZ100 group. These lipidomic changes were have been widely reported to be associated with macrophage inflammation. Therefore, our findings suggested that PM exposure induced disruption in lipid metabolism and classical activation in macrophages, resulting in a pro-inflammatory phenotype.

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

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:43

Chair: Sungju Yu (Ajou University)

Advanced Solution NMR Spectroscopy for Comprehensive Characterization of Crystalline Phases in Poly(vinylidene fluoride) (PVDF) for Good-performance Electrode

SeokKi Yun, Jiwon Kim[1], Quy Son Luu[1], Youngbok Lee[1,*]

DEPARTMENT OF CHEMICAL AND MOLECULAR ENGINEERING, Hanyang University, Korea

[1]*Department of Bionano Technology, Center for Bionano intelligence Education and Research, Hanyang University, Korea*

Poly (vinylidene fluoride) (PVDF) is a versatile dielectric polymer used in lithium-ion batteries and chemical equipment. It exists in four crystalline phases (α, β, γ and δ) with varying electrical responsiveness. Studies primarily focus on its efficiency as a binder through surface and electrochemical analyses but lack depth in examining cycling and polymorphic effects. In this study, we aim to develop a solution NMR-based technique for assessing the fine structure and crystallinity of PVDF materials, laying the foundation for high-performance PVDF binder material development and the establishment of a PVDF material database. As a first step, commercial PVDF samples were separated into α, β, and γ phases using various recrystallization techniques to gather information on their structure and crystallinity. The samples underwent recrystallization under varying solvent, drying temperature, heating rate, and drying gas conditions, and were analyzed via 1H and 19F NMR to determine their primary structures, including the presence of defects, and calculated H-T/H-H ratios. Subsequently, variable temperature-NMR experiments were conducted to observe temperature-dependent changes in the PVDF structure and crystallinity. After that, T1 and T1rho relaxation analyses were performed to assess the thermal stability and structural changes in the samples. Furthermore, to elucidate the detailed spatial structural information and the relationships between crystallinity phases (α, β, γ), analyses including 19F-19F selective COSY and 13C-19F HSQC were carried out. These research findings demonstrate the potential for effectively

utilizing solution NMR in evaluating the fine molecular structure and crystallinity of binder materials, which are directly linked to electrode performance.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Oral Presentation : **ANAL1.O-25**
Oral Presentation of Young Analytical Chemists
Room 214 THU 10:47
Chair: Sungju Yu (Ajou University)

Metabolic and immunological responses to Delta and Omicron variant infection in hamster lung tissue

Sunho Lee, Jueun Lee, Geum-Sook Hwang[1,*]

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

Coronavirus (COVID-19) has been continuously as an ongoing pandemic, with an increasing variety of viral variants emerging over time and shorter intervals between their appearances. The coronavirus directly infects the lungs, significantly impacting the immune system by modulating metabolic changes and triggering a cytokine storm. Additionally, various inflammatory cytokines are known to increase as the severity of coronavirus infections rises. However, the research on the relationship between virus infection-induced metabolic changes and the immune system is currently lacking.In this study, we performed metabolic profiling in hamster models using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS) to investigate metabolic changes after infection with the Delta and Omicron variants compared to pre-infection. The changes of cytokine levels derived from RNA sequencing data were examined to gain insights into their role in the immune response to SARS-CoV-2 variants. And then, we explored the associations between metabolic changes and inflammatory cytokines.In the metabolic profiles, arginine biosynthesis was significantly altered in both Delta and Omicron variants, while glutathione metabolism and tryptophan metabolism were significantly changed only in the Delta variant. For the alterations in cytokine levels, CCL5, CCL8, CSF1, and TNFAIP8L2 exhibited significant increases in both variant groups, whereas CCL4, CCL7, CXCL10, and IL-1β showed a substantial increase in the Delta group compared to the Omicron group. In the Delta variant, arginine exhibited significant positive correlations with CCL4 and CCL5, and proline and glutathione showed positive correlations with IL-12B. Glutathione oxidized displayed positive correlations with CCL7 and CCL8. In the Omicron variant, aspartate and ornithine were negatively correlated with CCL8 and TNFAIP8L2, respectively. In addition, proline exhibited negative association with CCL5 and CSF1 in the Omicron variant.These findings suggest that SARS-CoV-2 variant virus infections induce distinct metabolic changes and inflammatory responses, and changes in metabolic pathways can undergo modification due to the influence of the immune system within the lung of hamsters. This study can provide valuable insights into the altered metabolic pathways and immune system changes influenced by the Delta and Omicron variants.

Oral Presentation : **ANAL1.O-26**

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:51

Chair: Sungju Yu (Ajou University)

photoelectrocatalysis Effects of IrO_2 cocatalysts on $SrTiO_3$ nanocubes

Hyun Ju Yang, Jinju Kim, Je Hyun Bae*

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

Forming a heterojunction structure by loading a co-catalyst on the photocatalyst is one of the methods that can lead to the highest efficiency of the photocatalyst. $SrTiO_3$ with a cubic structure was prepared using a single-step hydrothermal method in this study. In addition, $IrO_2/SrTiO_3$ heterojunction structures were prepared by loading IrO_2 on the surface of $SrTiO_3$ by controlling the amount of Ir precursor through the impregnation method. The prepared material was analyzed using TEM(Transmission Electron Microscopy) to confirm the morphology, and it was observed that IrO_2 was well loaded on $SrTiO_3$ surface. In addition, the XPS (X-ray Photoelectron Spectroscopy) analysis result showed that IrO_2 clearly exists, as a peak value consistent with IrO_2 was observed at a specific binding energy. The photoelectrocatalytic activity of the synthesized nanocatalysts for photoelectrochemical water oxidation was investigated using linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS). It was confirmed that IrO_2 nanoparticles plays a good role as cocatalysts on the nanocubic $SrTiO_3$ surface for OER (Oxygen Evolution Reaction).

Oral Presentation : **ANAL1.O-27**

Oral Presentation of Young Analytical Chemists

Room 214 THU 10:55

Chair: Sungju Yu (Ajou University)

Voltage-programmed Capillary Gel Electrophoretic Separation for the Fast Screening of PCR Products of Severe Acute Respiratory Syndrome Coronavirus 2 with High Sensitivity

Changuk An, Seong Ho Kang[1,*]

Chemistry, Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Fast and highly sensitive detection has become essential to prevent the transmission of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). However, accelerating the analysis often leads to compromised precision and accuracy. This research aims to investigate a fast and highly sensitive screening technique for identifying polymerase chain reaction (PCR) products of SARS-CoV-2 using voltage-programmed capillary gel electrophoresis. By separating and identifying the PCR products related to the RNA-dependent RNA polymerase (RdRp) and spike (S) genes, we successfully diagnosed cases of coronavirus disease 2019 (COVID-19) within just 4 min using this method with strong dependability and precision. This indicates an acceleration of at least 7.5 times compared to previous COVID-19 diagnostic methods. The limit of detections for RdRp and S gene fragments were 1.34–3.46 pM. The developed approach is variously applicable, enabling the analysis of PCR products with specific DNA sizes and the identification of SARS-CoV-2 mutations without reducing resolution. Furthermore, it can also be applied to the fast analysis of DNA molecules associated with various infectious diseases.

Oral Presentation : **ANAL2.O-1**
Oral Presentation of Early-career Analytical Chemists
Room 214 FRI 09:00
Chair: Ji Won Ha (University of Ulsan)

Surface Modification of Fluorescent Nanodiamond for Their Applications

Haksung Jung

Quantum Technology Institute, Korea Research Institute of Standards and Science, Korea

Fluorescent nanodiamonds (FNDs) are attractive carbon nanoparticle due to their remarkable physicochemical properties. However, the low colloidal stability in salt aqueous buffer and the surface functionalization with different molecules of FND are still challenges for their applications. Here, I present the encapsulation strategy of FNDs into different structural polydopamine (PDA) shells (FND@PDA). Owing to diverse interaction of the PDA shells with different molecules, it permits secondary reaction via covalent and non-covalent interaction. I demonstrate different examples of PDA encapsulated FND using various functionalization approaches such as Michael addition reaction, hyperbranched polyglycerol growth, and noncovalent interaction. The functionalized FND@PDA can be employed as fluorescent probe, sensor and drug delivery vehicle. The robust PDA encapsulation strategy that I present provides an avenue for the development of FNDs as multifunctional labels, drug delivery vehicles, and targeting agents for biomedical applications.

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 09:15

Chair: Ji Won Ha (University of Ulsan)

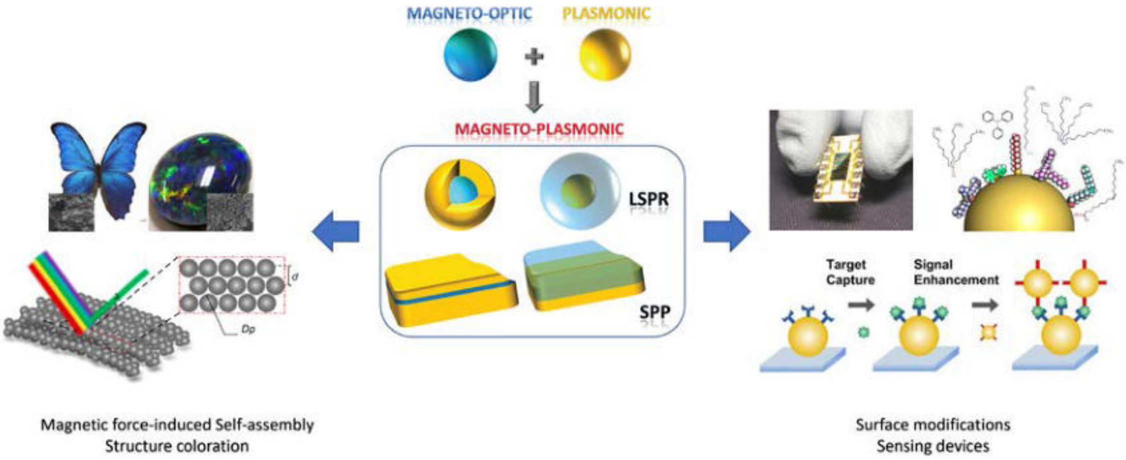
Emergence of Structural chirality and sensing capabilities from Magnetoplasmonic building blocks

Huu-Quang Nguyen, **Jaebeom Lee**[1,*]

Department of Chemistry, Chungnam National University, Korea

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

Chirality of matter as a field of science has spanned over 150 years since its discovery, and up until now, a vast range of both naturally-derived and artificial chiral materials have been extensively studied. Unlike the well-established basis of molecular chirality observed in simple organic molecules, the concept of structural chirality mainly revolves around the fabrication and self-assembly of nanosized structures, including metals, semiconductors, and other inorganic building blocks. In which, adaptations of Magneto-plasmonic (MagPlas) nanomaterials are surfacing as template-free strategies to compose optically active metasurfaces and superstructures that can achieve symmetry breaking and circular dichroism. Superstructures with chiral light manipulation capabilities are powerful tools for potential applications in photonics, biosensing, and nanoscale medicine. In this talk, current advances in this particular field of research will be discussed, including synthesis of zero- and one-dimensional MagPlas building blocks; self-assembly and incorporation of MagPlas nanomaterials into chirally active optical and sensing applications.


MAGNETO-OPTIC
PLASMONIC
MAGNETO-PLASMONIC
LSPR
SPP
d
Dp
Target Capture
Signal Enhancement
Magnetic force-induced Self-assembly
Structure coloration
Surface modifications
Sensing devices

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 09:30

Chair: Ji Won Ha (University of Ulsan)

Development of Multidimensional Analytical Platform for Characterization of Marine Polysaccharides based on LC/MS/MS

Nari Seo, Hyun Joo An[1,*]

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

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

Marine-derived polysaccharides are attracting considerable interests as high value-added industrial materials due to increased recognition of their potential benefits. Despite their significant functional attributes, research efforts have predominantly focused on exploring the functional properties of polysaccharides while neglecting the essential aspect of their structural characterization. Above all, understanding their structures remains an analytical challenge as they reveal classes of macro- and complex- molecules that share similar but imprecise monosaccharide composition, linkage position, and monomer arrangement. In this study, we have developed a groundbreaking analytical platform based on liquid chromatography-tandem mass spectrometry (LC-MS/MS) that could be an innovative means of elucidating the functional roles and improving quality of marine-derived polysaccharides. In addition, we successfully determined structure and content of fucoidan and alginic acid, which are functional polysaccharides from brown algae. Then, the correlation between their physicochemical properties and biological reactions was investigated, and furthermore, they assisted in the screening of raw materials. Our strategy presents a systematic and efficient approach for the characterization of the most dominant polysaccharides in nature, ultimately providing insight into applications as high value-added materials in fields such as food science, pharmaceuticals, cosmetics, and biomaterials.

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 09:45

Chair: Ji Won Ha (University of Ulsan)

Influence of Oxygen Plasma Treatment on the Electrocatalytic Activity of Single Gold Nanorods

Mukunthan Ramasamy, **Ji Won Ha**[1,*]

Department of Chemistry, University of Ulsan, India

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

When gold nanoparticles (AuNPs) interact with light, they exhibit the localized surface plasmon resonance (LSPR) phenomenon, which is the collective oscillation of surface free electrons. Gold nanorods (AuNRs) with broadly tunable optoelectronic properties driven by physical and chemical stimuli have gained considerable interest for a number of applications, including electrocatalysis and electrochemical sensing. The LSPR properties of AuNRs are influenced by changes in size, shape, composition, and refractive index (RI) of the surrounding medium. Oxygen plasma consisting of high intensities of energized electrons and ions has been used in our experiment to stimulate the catalytic property of AuNRs. In this work, AuNRs have been immobilized on ITO substrates and exposed to varying oxygen plasma periods. We discuss the spectral, structural, and electrocatalytic activity of AuNRs exposed to oxygen plasma using dark-field scattering (DFS) microscopy and spectroscopy, scanning electron microscopy (SEM), and cyclic voltammetry (CV). Furthermore, we discuss the electrocatalytic activity of oxygen plasma-treated AuNRs and its potential-dependent plasmonic effect at the single-particle level.Keywords: gold nanorods, oxygen plasma, localized surface plasmon resonances, electrocatalysis

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 10:00

Chair: Ji Won Ha (University of Ulsan)

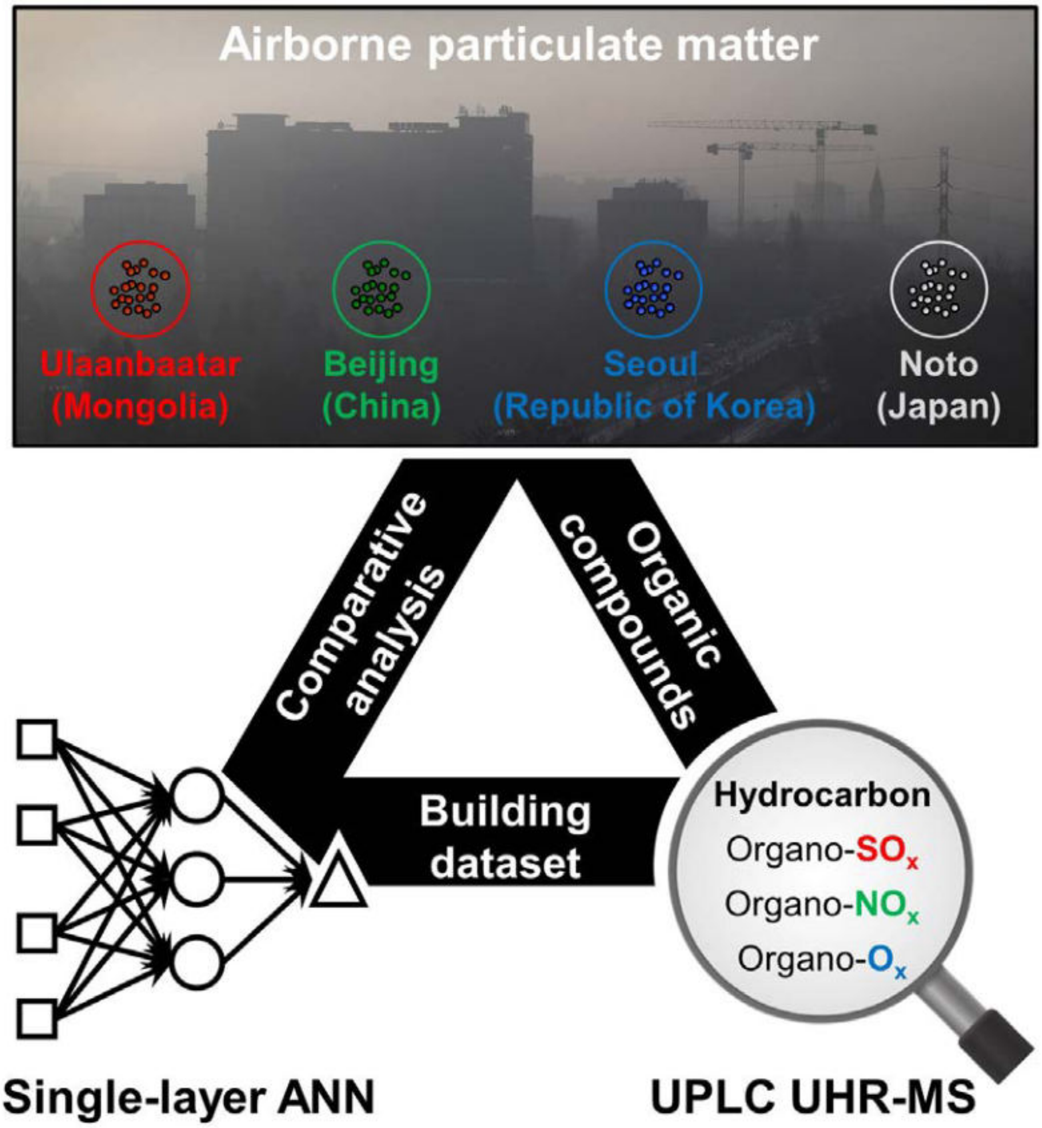
Evaluating seasonal differences in organic chemical constituents of airborne particulate matter in Ulaanbaatar, Beijing, Seoul, and Noto using UPLC-FT-ICR MS and artificial neural network

Seungwoo Son, Young Hwan Kim[1,*], Sunghwan Kim[*]

Department of Chemistry, Kyungpook National University, Korea

[1]*Center for Research Equipment, Korea Basic Science Institute, Korea*

Airborne particulate matter (PM) is a significant environmental pollutant, with increasing concentrations annually. PM affects health, so it is important to understand PM and its effects. In this study, analysis with high-throughput ultra-performance liquid chromatography (UPLC) coupled with atmospheric pressure chemical ionization (APCI) fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) and an artificial neural network (ANN) was performed for PM$_{2.5}$ (aerodynamic diameter $\leq$ 2.5 *μm*) samples collected in four sites by season. A total of 350 PM$_{2.5}$ samples were analyzed, collected daily during spring, summer, and winter in Ulaanbaatar, Beijing, Seoul, and Noto. The ANN modeling correlated UPLC (-)APCI FT-ICR MS data with season, identifying chemicals contributing to season at each site. The ANN model was evaluated with a back-propagation neural network (BPNN) and confirmed to work well. Data with a high seasonal contribution of PM$_{2.5}$ in each site were extracted through the ANN, and Van Krevelen diagram and class distribution analysis were performed. The results showed that Ulaanbaatar's winter PM$_{2.5}$ was mainly composed of SO_x and aromatic compounds, indicating coal combustion as the primary source. Beijing and Seoul were identified as high contributors of aromatic compounds to winter PM$_{2.5}$, which were thought to be related to petroleum combustion, such as heating. The correlation analysis using the ANN is expected to provide detailed molecular level information on seasonal contributing chemicals in the vast data and can be used for secondary organic aerosol generation contribution analysis.


Airborne particulate matter
Ulaanbaatar (Mongolia)
Beijing (China)
Seoul (Republic of Korea)
Noto (Japan)
Comparative analysis
Organic compounds
Building dataset
Hydrocarbon
Organo-SO_x
Organo-NO_x
Organo-O_x
Single-layer ANN
UPLC UHR-MS

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 10:15

Chair: Ji Won Ha (University of Ulsan)

The Artificial Circulatory System for Tumoroids (ACT): Investigating the Impact of Pharmaceutical and Biomimetic Approaches on through MS-based Analysis

Sooyeon Chae, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Personalized cancer medicine relies on tailored treatments guided by precise scientific evidence encompassing pharmaceuticals, genes, proteins, and metabolites. Essential to this endeavor is the identification of robust biomarkers for individualized therapy.Recent research has highlighted the critical interplay between pharmacokinetics, cell biology-pharmacodynamics, and fluid mechanics within the body's circulatory system. Conventional laboratory cell-based models have fallen short in integrating these factors, leading to inconsistent drug efficacy and biomarker identification in clinical trials. Bridging this gap requires innovative pharmaceutical and biomimetic models that account for fluidic conditions.To address these challenges, we introduce the Artificial Circulatory Tumor (ACT) system, a versatile platform enabling mass spectrometry-based investigations. ACT leverages pharmacokinetic software, computer-aided design (CAD), and advanced fluid systems to construct biomimetic environments.Our study employs cutting-edge analytical techniques, including mass spectrometry (MS), computational fluid dynamics (CFD), and spectroscopy, to demonstrate the ACT's ability to replicate biomimetic pharmacodynamics. Our findings offer crucial insights into personalized cancer medicine, showcasing the ACT system's potential in biomarker discovery. By transcending the limitations of traditional laboratory models, ACT promises to expedite the development of personalized cancer treatments.

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 10:30

Chair: Ji Won Ha (University of Ulsan)

An Active Interface for High Performance Olivine Cathode Materials

Dung Nguyen, Jimin Kim[1], Youngil Lee[1,*]

Chemical Industry Research Institute, Core Research Institute, University of Ulsan, Korea

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

Increasing energy density and fast charging capability with higher energy utilization have been considered critical for electric vehicles to be commonly accepted. As the source of Li ions, the cathode is a vital component of LIBs. The battery energy critically depends on how the Li ions in the cathode are utilized, especially how they migrate from bulk toward the particle surface and vice versa during charge and discharge. Our recent work has demonstrated that the electrochemical performance of the interfacial structures of cathode materials, as a confined region where the charge transfer initially takes place, strongly influences the overall performance of the active materials. The construction of fast Li ion and electron channels on the olivine particles is the key solution to achieve excellent cathodes. In this study, a hybrid conductive coating layer consisting of carbon (C) and $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) solid electrolyte has been applied on various olivine-type materials, including $LiFePO_4$ (LFP), $LiFe_{0.4}Mn_{0.6}PO_4$ (LFMP), and $LiFe_{0.4}Mn_{0.3}Co_{0.3}PO_4$ (LFMCP), to take advantage of each coating component. Such an arrangement enhances the conductivity of both the Li ions and the electrons to significantly improve the insertion/extraction of the Li-ions into/from the surface to the core of the active material particles. The hybrid coating enables us to achieve promising high voltage, high energy density, and high rate capability active materials with decent cycling stability. We believe that our established principles could universally apply to other electrode materials that have been the frontiers of new battery chemistries.

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

Oral Presentation of Early-career Analytical Chemists

Room 214 FRI 10:45

Chair: Ji Won Ha (University of Ulsan)

Photo-reversible Tuning of Chemical Interface Damping in Single Gold-nanorods by Aminoazobenzene

Jaeran Lee, Ji Won Ha[*]

Department of Chemistry, University of Ulsan, Korea

Recently, chemical interface damping (CID) has been proposed as a new plasmon damping pathway based on interfacial hot-electron transfer from metal to adsorbate molecules. It has been considered essential due to its potential impact on efficient photochemical processes and sensing experiments. However, thus far, studies focusing on controlling CID in single gold nanoparticles have been very limited, and in situ reversible tuning has remained a considerable challenge. In this study, we investigated the process of CID upon adsorption of aminoazobenzene, whose photo-reversible molecular structure is well known, onto gold nanorods using total internal reflection dark-field microscopy, and controlled the structure of the adsorbate aminoazobenzene by UV(365 nm)/Vis(465 nm) switching irradiation. By analyzing the red and blue shift of localized surface plasmon resonance (LSPR) peak and the linewidth change according to the cis-trans form conversion, it was confirmed that CID was controlled by inducing changes in the adsorbate molecules without changing the refractive index, pH and temperature of the solution. Furthermore, in the interaction of aminoazobenzene and cucurbit[8]uril, the binding in trans-form and separation in cis form between the two molecules suggested the non-contact and reversible applications of capsules based on AuNRs.

Award Lecture in Division : **LIFE.O-7**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 10:20

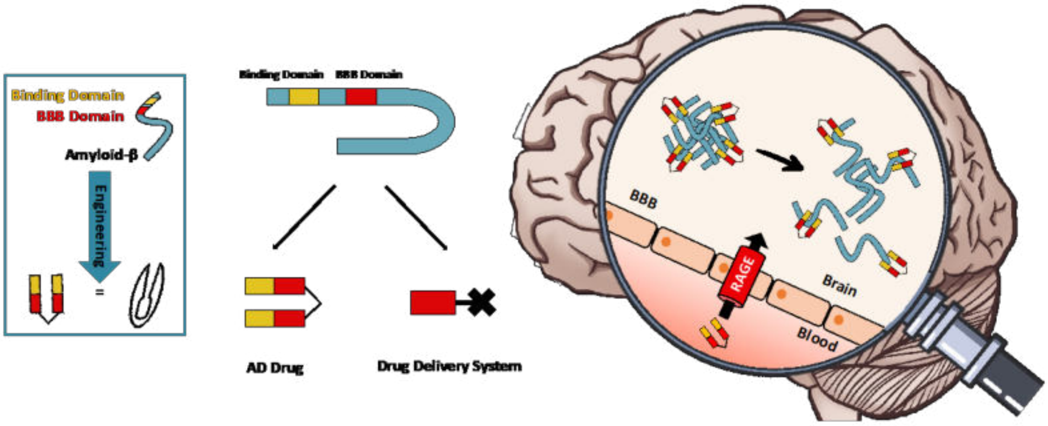
Chair: Kwang Yeon Hwang (Korea University)

Chemical-Driven Clearance of Misfolded Proteins for Alzheimer's Disease Drug Discovery by Dimeric Amyloid Fragments

YoungSoo Kim

Department of Pharmacy, College of Pharmacy, Korea

Amyloid-β (Aβ) in the form of neurotoxic aggregates is regarded as the main pathological initiator and key therapeutic target of Alzheimer's disease. However, anti-Aβ drug development has been impeded by the lack of a target needed for structure-based drug design and low permeability of the blood–brain barrier (BBB). An attractive therapeutic strategy is the development of amyloid-based anti-Aβ peptidomimetics that exploit the self-assembling nature of Aβ and penetrate the BBB. Herein, we designed a dimeric peptide drug candidate based on the N-terminal fragment of Aβ, DAB, found to cross the BBB and solubilize Aβ oligomers and fibrils. Administration of DAB reduced amyloid burden in 5XFAD mice, and downregulated neuroinflammation and prevented memory impairment in the Y-maze test. Peptide mapping assays and molecular docking studies were utilized to elucidate DAB-Aβ interaction. To further understand the active regions of DAB, we assessed the dissociative activity of DAB with sequence modifications.


Binding Domain
BBB Domain
Amyloid-β
Engineering
Binding Domain
BBB Domain
AD Drug
Drug Delivery System
BBB
RAGE
Brain
Blood

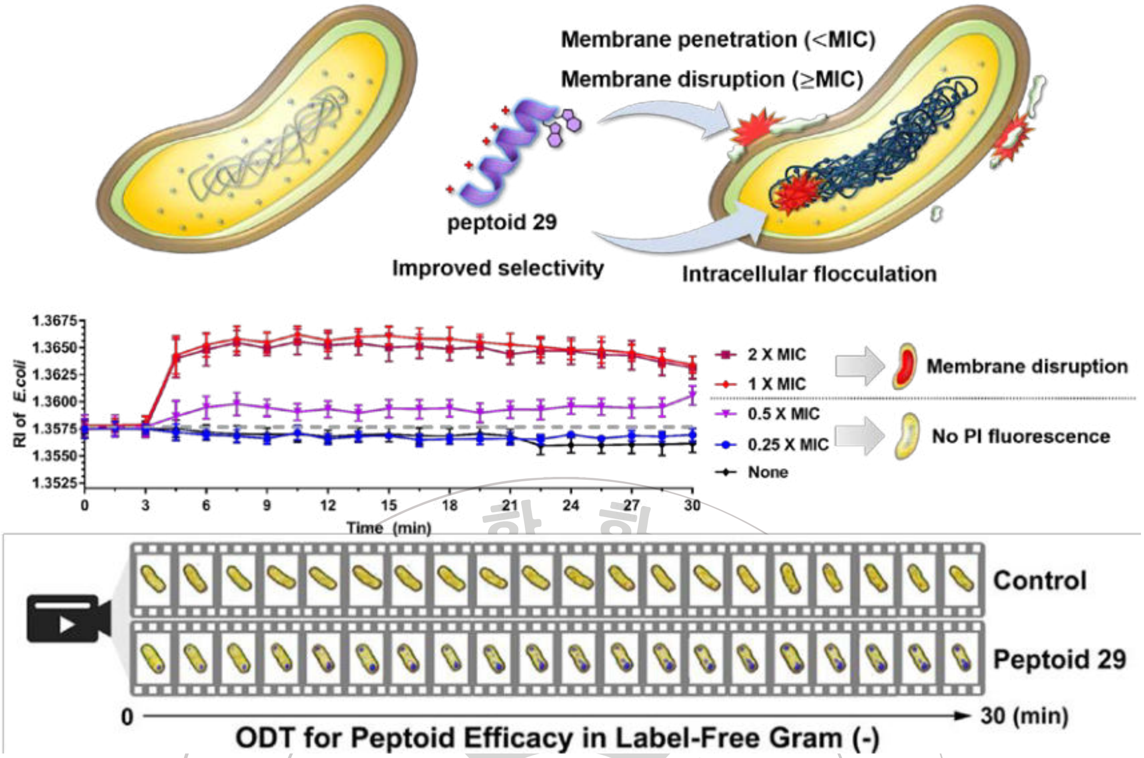
Oral Presentation : **LIFE.O-1**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 304+305+306 THU 09:00
Chair: Min Hee Lee (Sookmyung Women's University)

Multi-target mechanism of antimicrobial peptoids: real-time and label-free monitoring of bacterial morphological changes by three diementional optical diffraction tomography

Minsang Kim, Jiwon Seo[*]

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

Antimicrobial peptides (AMPs) are have been spotlighted as promising antibiotic agents against broad-spectrum pathogens. Peptoids with *N*-substituted glycines backbone, which mimic the structure of AMPs, have been utilized for antimicrobials because of their resistance against proteolysis. Primary bactericidal mechanism of peptoids are generally known to membrane disruption; however, non-specific aggregation of intracellular components also suggested as an important antimicrobial mechanism, which was directly associated with fast killing kinetics. Here, we investigated structure-activity relationship (SAR) of a library of indole side chain-containing peptoids, designed to specifically interact with bacterial membrane, providing peptoid 29 as a hit compound. Then, we performed the quantitative morphological analysis of live bacterial cells treated with AMPs and peptoid 29 in a label-free manner using 3D optical diffraction tomography (ODT). We unambiguously demonstrated that both membrane disruption and intracellular biomass flocculation were primary mechanisms of bacterial killing by real-time monitoring morphological changes of bacteria. These multi-target mechanisms and rapid drug action could be a merit for the discovery of a resistance-breaking novel antibiotic drug.


Membrane penetration (<MIC)
Membrane disruption (≥MIC)
peptoid 29
Improved selectivity
Intracellular flocculation
RI of E.coli
1.3675
1.3650
1.3625
1.3600
1.3575
1.3550
1.3525
0
3
6
9
12
15
18
21
24
27
30
Time (min)
2 X MIC
1 X MIC
0.5 X MIC
0.25 X MIC
None
Membrane disruption
No PI fluorescence
Control
Peptoid 29
0
30 (min)
ODT for Peptoid Efficacy in Label-Free Gram (-)

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 09:12

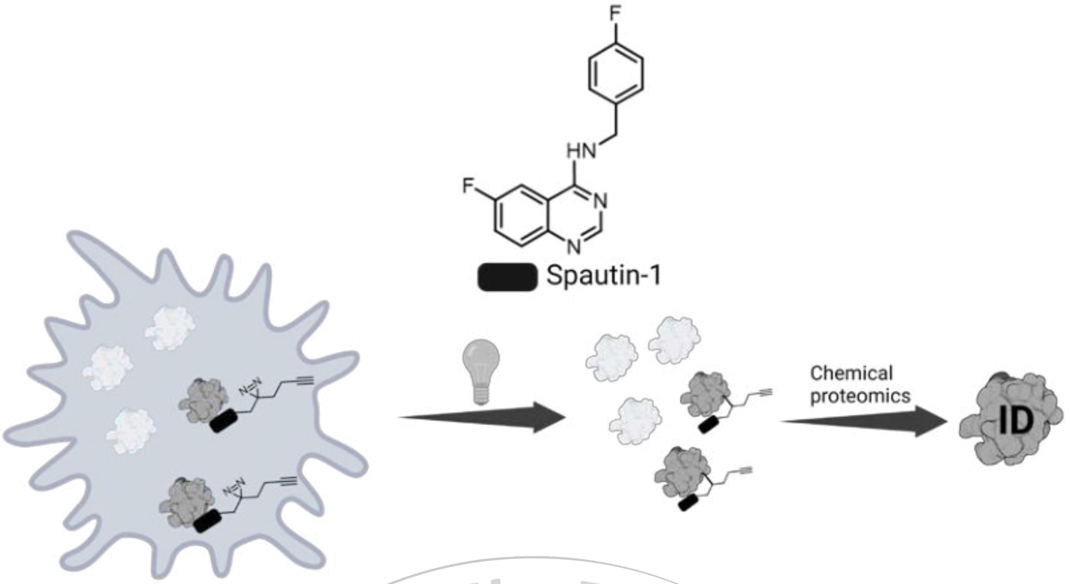
Chair: Min Hee Lee (Sookmyung Women's University)

Photo-Spautin for cellular functional target identification

Kostiantyn Kozoriz, Jun-Seok Lee*

Department of Pharmacology, Korea University, Korea

Autophagy, a cellular housecleaning and self-renewal process, plays a critical role in neurodegenerative diseases, cancer, and more. Despite significant advancements in autophagy research, epitomized by the 2016 Nobel Prize for the discovery of autophagy genes, the clinical translation of autophagy modulators remains limited. Spautin-1, a potent small-molecule inhibitor of autophagy, has shown promise in preclinical models by inhibiting ubiquitin-specific peptidases USP10 and USP13, thereby promoting the degradation of the Beclin1 subunit of Vps34 PI3 kinase complexes. Nevertheless, the full spectrum of Spautin-1's biological activities, including its off-target effects, has not been completely elucidated. This is a crucial gap that must be addressed before Spautin-1 can advance to clinical trials. In this study, we introduce novel photoaffinity probes based on Spautin-1, incorporating a diazirine photoaffinity label and an alkyne enrichment handle. These probes are designed to mimic Spautin-1's biological activity, facilitating target identification through chemical proteomics. Our work aims to unveil the molecular targets of Spautin-1 and to provide valuable insights into its mechanism of action and safety profile. The probes also have potential applications in live-cell labeling experiments to validate subcellular localization and target engagement. Our findings are expected to significantly advance our understanding of Spautin-1's mode of action and could guide the development of safer and more specific Spautin-1 analogs for therapeutic applications.


F
HN
N
N
F
Spautin-1
N=N
Chemical
proteomics
ID

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 09:24

Chair: Min Hee Lee (Sookmyung Women's University)

Fmoc-amino acid as a minimal molecular scaffold for liquid-liquid phase separation

Hyo Jae Jeon, Kyungtae Kang[1,*]

Chemistry, Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Liquid-liquid phase separation (LLPS) is intricately linked to numerous cellular phenomena, encompassing stress response, signal transduction, gene expression, and protein aggregation. Despite its significance, the underlying molecular mechanisms of LLPS remain partially elucidated. The establishment of a collection of fundamental molecular frameworks for systematic investigation of LLPS would be immensely valuable for comprehending and harnessing LLPS. Within this research endeavor, we scrutinized the LLPS behaviors of Fmoc-protected amino acids. Fmoc-amino acids have long been subject to investigation due to their fibrogenetic properties; however, their propensity for LLPS has yet to be reported. Our findings indicate that a substantial proportion of Fmoc-amino acids exhibit LLPS phenomena, contingent upon the pH and ionic strength of the solution. We systematically probed the conditions under which each Fmoc-amino acid undergoes LLPS, subsequently demonstrating that the formation of liquid coacervates comprising Fmoc-amino acids holds potential for diverse biomolecular enrichment or organic reaction catalysis.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 09:36

Chair: Min Hee Lee (Sookmyung Women's University)

Discovery of novel small molecule inhibitors targeting HIF-2α

Yeonju Song, Yeonjin Ko*

Korea Institute of Science and Technology, Korea

Clear cell renal cell carcinoma (ccRCC) is a leading cause of mortality in kidney cancer patients, characterized by somatic mutations in the von Hippel-Lindau (VHL) tumor suppressor gene. Dysfunctional pVHL leads to the accumulation of hypoxia-inducible factor-2α (HIF-2α), promoting the formation of HIF-2α/HIF-1β heterodimeric transcription factors. This complex orchestrates the expression of target genes involved in angiogenesis, glucose metabolism, and erythropoiesis. Targeting the interaction between HIF-2α and HIF-1β holds promise for ccRCC treatment; Belzutifan (PT2977) is the sole FDA-approved small molecule targeting this pathway. However, drug resistance related to the HIF-2α G323E mutation arises during prolonged treatment with analogs like PT2385 and PT2399, necessitating innovative strategies to overcome this challenge. In this study, we synthesized a library of 132 small molecules designed to engage the hydrophobic cavity of the HIF-2α PAS-B domain. Through a cell-based luciferase reporter assay, we identified seven compounds with superior efficacy against HIF-2 transcriptional activity compared to PT2385. Notably, this efficacy persists despite resistance mutations. Further biophysical and biochemical assays revealed that compound C-7 disrupts HIF-2α/HIF-1β heterodimers and downregulates HIF-2 target genes in cells expressing wild-type HIF-2α or the HIF-2α G323E mutant. Collectively, this study discovers novel small molecule scaffolds for HIF-2α inhibitors, expanding potential therapeutic strategies for HIF-2α-driven tumors.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 09:48

Chair: Min Hee Lee (Sookmyung Women's University)

[Withdrawal] Revealing new phosphoarginine binding proteins using chemoproteomic methods

Seungmin Ahn, Jung-Min Kee*

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

- Withdrawal -

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 304+305+306 THU 10:00

Chair: Min Hee Lee (Sookmyung Women's University)

Indolizine-based fluorescent compounds array for noninvasive monitoring of glucose in bio-fluids using on-device machine learning

Eunsu Kim, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Introducing an innovative paper-based portable assay system for accurate glucose level monitoring in tears. This system integrates enzyme reactions, fluorescence properties, and machine learning algorithms to achieve precision. By printing wax on cellulose paper, melting it to form test zones, and depositing fluorescent compounds and glucose oxidase, a unique fluorescence pattern specific to glucose concentration is generated. Capillary action from a small sample drop evenly distributes the sample, initiating the pattern. Image data from the fluorescent compounds array is analyzed by two models. The first, a random forest model, categorizes concentrations discretely based on training data granularity. The second, an SVM regression model, estimates glucose concentration with finer granularity. These models, coupled with feature engineering, enable efficient sensor data processing on resource-limited mobile platforms. The random forest yields remarkable accuracy, classifying glucose concentrations with up to 96.7% accuracy (at 0.2 mM intervals, MSE of 0.060 mM), and the SVM regression model results in an MSE of 0.026 mM. This novel, cost-effective paper-based system holds potential as a noninvasive method for diabetes management through tear glucose level monitoring.

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

Oral Presentations for Young Scholars in Organic Division

Convention Hall 2 THU 09:00

Chair: Isaac Choi (Chungbuk National University)

Synthesis and Photophysical Properties of Diaminobenzene-based Simple Fluorophores

Dopil Kim, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Small molecule fluorophores have been widely studied for various applications such as organic light emitting diodes (OLED) and molecular probes. Especially, in single benzene-based fluorophores (SBBF) with multiple electron-donating groups (EDGs) and electron-withdrawing groups (EWGs), a variety of photophysical properties have been developed through adjusting the combination and positions of functional groups.[1,2,3] Not only for the electronic characters, but also the structural and positional features are important for their photophysical properties.

In this presentation, we will discuss the synthesis and photophysical properties of diamino terephthalate-based fluorophores. Two amino groups work for EDGs and two ester groups serve for EWGs in our system, and the additional functional group controls have been attempted. Therefore, the electronic effect of amine derivatives along with their structural effects will be discussed.

References

1 Kim, H.; Park, W.; Kim, Y.; Filatov, M.; Choi, C. H.; Lee, D. *Nat. Commun.* 2021, *12*, 5409.

2 Sarkar, S., Shil, A., Jun, Y. W., Yang, Y. J., Choi, W., Singha, S., Ahn, K. H., *Adv. Funct. Mater.* 2023, 2304507.

3 Kim, J.; Oh, J. H.; Kim, D. *Org. Biomol. Chem.* 2021, *19*, 933.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentations for Young Scholars in Organic Division

Convention Hall 2 THU 09:15

Chair: Isaac Choi (Chungbuk National University)

Regioselective etherifications of quercetin and their fluorescent properties

Yongju Kim[*], Yerim Kim

Korea University, Korea

Quercetin contains several hydroxy groups (OH) at different positions on its molecular structure, including positions 3, 5, 7, 3', and 4'. The regioselective reaction of a hydroxy group in quercetin and the study of the related physical properties remain challenging. Herein, we report the regioselective etherification of quercetin derivatives, wherein the oligoether chains were linked to provide quercetin derivatives. Interestingly, the penta-substituted quercetin derivative exhibited a higher fluorescence intensity than the tetra-substituted one. The fluorescence behavior of synthetic derivatives was investigated using solvatochromism, molecular aggregations, computational calculations, and hydrogen bonds with solvents. The fluorescent penta-substituted quercetin derivative did not show any cytotoxicity up to 600 μM concentration and hence is a novel biocompatible fluorescent molecule.

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

Oral Presentations for Young Scholars in Organic Division

Convention Hall 2 THU 09:30

Chair: Isaac Choi (Chungbuk National University)

A non-toxic fluorescent probe for real-time visualization of glioblastoma and its clinical application

Jaehoon Kim, Dokyoung Kim[1,*]

Department of Biomedical Science Graduate School , Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Fluorescence-guided surgery (FSG) is a surgical method that uses a tumor-specific fluorescent probe to selectively visualize the tumor area in the operating room. It has been mainly used for brain tumor surgery that is difficult to distinguish from normal tissue, such as glioblastoma (GBM). FGS is an important tool for GBM surgery, but the fluorescent probes for FGS developed so far have been accompanied by serious side effects. To address these side effects, we reported reaction-based fluorescent probes based on 4-chloro-7-nitrobenzofurazan (NBD) fluorophore capable of detecting cysteine (Cys) and homocysteine (Hcy), which are biomarkers of GBM, and their applications in previous studies. However, it was confirmed that our probes showed a cytotoxicity problem in the leaving group (L.G.) formed after the reaction between the fluorescent probe and the analytes. In order to overcome these problems, in this study, we disclosed a non-toxic fluorescent probe for detecting biothiols and its clinical application for real-time visualization of human GBM. To develop a non-toxic fluorescent probe, we systematically performed toxicity analysis in several cell lines of various L.G., and among them, 2-hydroxy-pyridine showed negligible toxicity. In addition, NPO-o-Pyr, a fluorescent probe derivative based on 2-hydroxy-pyridine, showed high specificity and sensitivity (LOD: 0.071 ppm for Cys; 0.189 ppm for Hcy), fast response time (

Oral Presentation : **ORGN.O-4**
Oral Presentations for Young Scholars in Organic Division
Convention Hall 2 THU 09:45
Chair: Isaac Choi (Chungbuk National University)

Copper(I)-Catalyzed Decarboxylative Nitrogen–Phosphorus Bond Formation:Preparation of *N*-Acyl Iminophosphoranes

Jinhwan Park, Anattil Unnikrishnan Krishnapriya[1], Yeongmi Park, Minsuk Kim, Tyler W. Reidl[2], Rositha Kuniyl[1], Jongwoo Son[3,*]

Department of Chemical Engineering (BK21 FOUR Graduate Program), Dong-A University, Korea
[1]*Department of Chemistry, Indian Institute of Technology-Palakkad, India*
[2]*Department of Research, Development & Innovation, Evonik Industries, United States*
[3]*Department of Chemistry, Dong-A University, Korea*

Iminophosphoranes are versatile intermediates, which constitute nitrogen–phosphorus double bond and can serve as important feedstocks for various organic transformations in natural product synthesis, drug discovery, and functional materials. Herein, we report a sustainable synthetic protocol for *N*-acyl iminophosphoranes employing dioxazolones and phosphines in copper(I) catalysis. This practical approach delineates an atom-economic fashion using dioxazolones, only generating carbon dioxide as a byproduct and excellent functional group tolerance for diverse dioxazolones and phosphines. Additionally, we implemented transformation of *N*-acyl iminophosphoranes to useful synthetic motifs such as nitriles and primary amides. Finally, we also performed DFT calculation and several mechanistic studies to delineate a plausible reaction mechanism.

Oral Presentation : **ORGN.O-5**
Oral Presentations for Young Scholars in Organic Division
Convention Hall 2 THU 10:00
Chair: Isaac Choi (Chungbuk National University)

Axial Coordination-driven Construction of Porphyrin-based Three-Dimensional Hydrogen-Bonded Organic Frameworks

Hyunjun Park, **Woo-Dong Jang**[1,*]

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

Among the porous materials, Hydrogen-bonded Organic Frameworks (HOFs) are an emerging class of crystalline materials. Due to H-bond's flexible and reversible nature, HOFs typically feature facile synthesis under mild conditions, solution processability, and easy recyclability via simple recrystallization. However, the preparation of HOFs with high permanent porosity is still more challenging than MOFs and COFs due to the weak interaction of hydrogen bonds than coordination bonds and covalent bonds. To achieve stable open framework structures with highly porous, several strategies have been attempted. In this study, we prepare porphyrin-based HOFs (YSH-8M) using four different metalloporphyrins (5,10,15,20-tetrakis(3,5-dicarboxyphenyl) porphyrins; OCTPPM, M = Zn, Co, Ni and Pt). The Zinc and Cobalt porphyrins are known to form axially 5 or 6 coordination with N- or O- donor guests. While the Nickel and Platinum porphyrins with low spin d8 configuration predominantly form square planar without axial coordination complex. The Single Crystal X-ray Diffraction (SC-XRD) revealed the structural difference of YSH-8M. In addition, each activated YSH-8M showed drastically different porosity. Activated YSH-8Zn, which has the highest BET surface area value (1665 m2/g), affords outstanding performance in gas separation from binary and tertiary mixtures of C1, C2, and C3 alkanes.

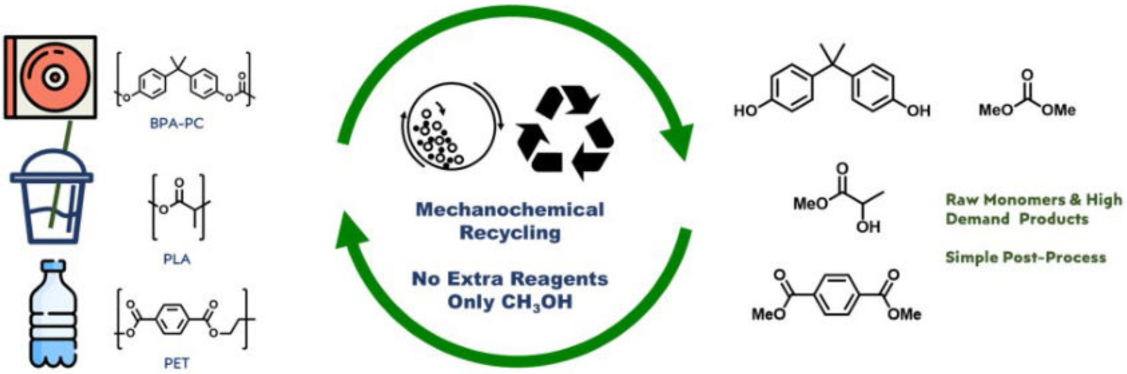
Oral Presentation : **ORGN.O-6**
Oral Presentations for Young Scholars in Organic Division
Convention Hall 2 THU 10:15
Chair: Isaac Choi (Chungbuk National University)

Chemical Recycling of Polycarbonate and Polyester without Solvent and Catalyst: Mechanochemical Methanolysis

HyoWon Lee, Jeung Gon Kim[1,*]

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

We present a green and economical approach to chemical recycling of commercial polycarbonates and polyesters, specifically poly(bisphenol A carbonate), poly(ethylene terephthalate), and poly(lactic acid). Our method involves mechanochemical ball-milling of a heterogeneous mixture of plastic and methanol, resulting in quantitative depolymerization to yield monomers or useful chemical units that already have high demands. We found that the energy-intensive step is forming physical contact between the reactants, rather than the chemical methanolysis itself. Mechanochemical ball-milling facilitates sufficient physical contact and energy transfer between plastics and methanol, eliminating the need for solvents and catalysts. Our study demonstrates a practical and sustainable process with minimal chemical input and simple output for the chemical recycling of these plastics.



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

Oral Presentations for Young Scholars in Organic Division

Convention Hall 2 THU 10:30

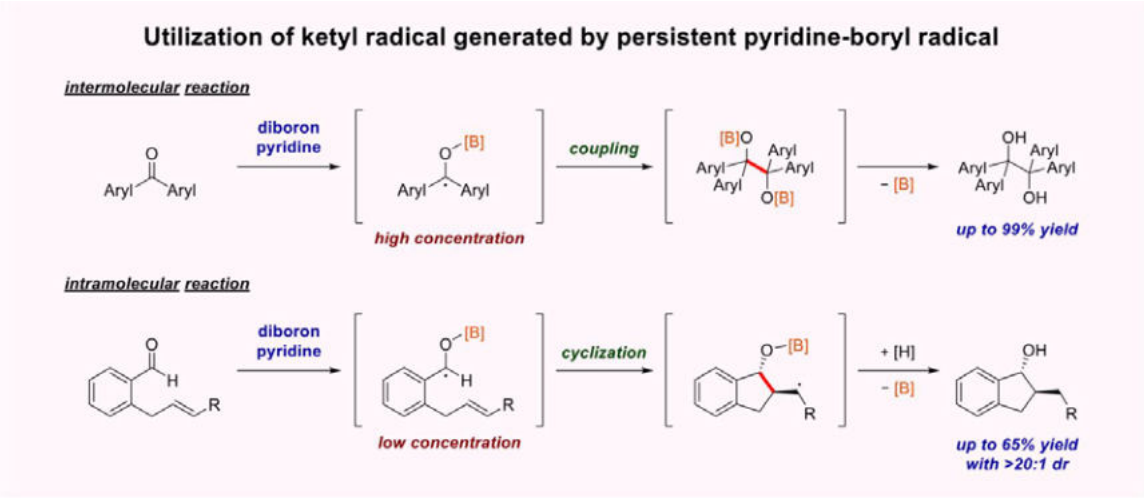
Chair: Isaac Choi (Chungbuk National University)

Utilization of ketyl radical generated by persistent pyridine-boryl radical on pinacol coupling of diaryl ketones and cyclization of 2-allylic benzaldehydes

Junhyuk Jo, Won-jin Chung*

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

While studying direct functionalization of flavone with persistent pyridine-boryl radical, an unexpected dimerization of flavone into 1,2-diol was observed. The generation of ketyl radical by diboron in the presence of pyridine catalyst was known, but its dimerization had not been reported. Investigations of the optimal conditions and substrate scope revealed that diaryl ketone was superior to monoaryl carbonyl compounds. Under the optimized reaction conditions, benzopinacols were obtained up to 99% yield. In addition, it was rationalized via DFT calculation that both aromatic rings were required for the stabilization of the transition state at the ketyl radical generation step. Subsequently, the reaction conditions with aromatic aldehyde were also surveyed, but hydrobenzoin was produced in only 59% yield with 1:1 dr. Because it was speculated that the intermolecular coupling of aromatic aldehyde suffered from the low concentration of the ketyl radical, an intramolecular reaction was evaluated for more efficient utilization of the generated ketyl radical. Therefore, a diastereoselective indanol synthesis was developed via introduction of an allylic group to the aromatic ring of the aldehyde. Gratifyingly, *trans*-indanols were obatained in up to 65% yield with >20:1 dr after column chromatography. The optimal combination of the diboron reagent and the substrate for high diastereoselection was rationalized by DFT calculation.


Utilization of ketyl radical generated by persistent pyridine-boryl radical
intermolecular reaction
O
Aryl
Aryl
diboron
pyridine
O
[B]
Aryl
Aryl
high concentration
coupling
[B]O
Aryl
Aryl
Aryl
Aryl
O[B]
- [B]
OH
Aryl
Aryl
Aryl
Aryl
OH
up to 99% yield
intramolecular reaction
O
H
R
diboron
pyridine
O
[B]
H
R
low concentration
cyclization
O
[B]
R
+ [H]
- [B]
OH
R
up to 65% yield
with >20:1 dr

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

Oral Presentations for Young Scholars in Organic Division

Convention Hall 2 THU 10:45

Chair: Isaac Choi (Chungbuk National University)

One-Carbon Homologative Lactonization as Step-Economical Routes to γ-Butyrolactones

Hosam Choi

Chemistry, The Catholic University of Korea, Korea

Natural products with gamma lactone as their main skeleton have a wide and excellent potential physiological activity effect such as anticancer, antibiotics, anti-bacteria, anti-malaria, and anti-fungi. Due to this variety of therapeutic usefulness, a synthetic approach toward the mirror image selectivity structure of gamma lactone has been developed. Successful synthesis methods are significantly limited in terms of substrate range diversity, location and stereochemical selectivity, and availability of easy starting materials. In addition, to date, many asymmetric synthesis methods have focused on the generation of one stereoscopic center, and strategies for providing optically active gamma-lactone synthesis with two stereoscopic centers are very limited. Recognizing these shortcomings, this lab improved the Kowalski ester homologation reaction using an aldol substrate that can be easily synthesized through chiral aids, conducted a cis/trans-gamma lactone skeleton synthesis study with two stereoscopic centers maintained by a single reaction. Recognizing these shortcomings, this laboratory improved the Kowalski ester homologation reaction using an aldol substrate that can be easily synthesized through chiral auxiliary, and conducted a cis/trans-gamma lactone skeleton synthesis study centered on two stereoscopes maintained by a single reaction. Furthermore, gamma lactone synthesis was performed using a photo reaction through the formation of a nickel-carbene intermediate as a one-step reaction. In this presentation, I would like to introduce the study.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 09:00

Chair: Jonghoon Kim (Soongsil University)

Optimization and evaluation of pyridinyl vinyl sulfones as Nrf2 activator for the antioxidant and anti-inflammatory effects

Byungeun Kim, **Ki Duk Park**[1,*]

Bio-Medical Science & Technology, University of Science and Technology, Korea

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

Many studies have reported that chalcone-based compounds exhibit biological activities such as anticancer, antioxidant, anti-inflammatory and neuroprotective effects. Among the published chalcone derivatives, (E)-1-(3-methoxypyridin-2-yl)-3-(2-(trifluoromethyl)phenyl)prop-2-en-1-one (VEDA-1209), which is currently undergoing preclinical study, was selected as a starting compound for the development of new nuclear factor erythroid 2-related factor 2 (Nrf2) activators. Based on our previous knowledge, we attempted to redesign and synthesize VEDA-1209 derivatives by introducing the pyridine ring and sulfone moiety to ameliorate its Nrf2 efficacy and drug-like properties. Among the synthesized compounds, (E)-3-chloro-2-(2-((3-methoxypyridin-2-yl)sulfonyl)vinyl) pyridine (10e) was found to have approximately 16-folds higher Nrf2 activating effects than VEDA-1209 (10e: EC50 = 37.9 nM vs VEDA-1209: EC50 = 625 nM) in functional cell-based assay. In addition, 10e effectively improved drug-like properties such as CYP inhibition probability and metabolic stability. Finally, 10e demonstrated excellent antioxidant and anti-inflammatory effects in BV-2 microglial cells and significantly restored spatial memory deficits in lipopolysaccharide (LPS)-induced neuroinflammatory mouse models.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 09:12

Chair: Jonghoon Kim (Soongsil University)

Discovery of a SARS-CoV-2 Nsp1 Inhibitor for Broad-Spectrum Therapeutics Against SARS-CoV-2 Variants

Wan Gi Byun, **Seung Bum Park***

Department of Chemistry, Seoul National University, Korea

The ongoing COVID-19 caused by SARS-CoV-2 has been extended by new variants of concerns like Omicron, known for its increased transmissibility. These variants mutate rapidly, casting doubt on the effectiveness of existing COVID-19 vaccines. This underscores the need for effective treatments capable of countering a range of variants and viruses. SARS-CoV-2 Nsp1 hampers host defense mechanisms and contributes to pathogenicity by directly blocking the host ribosomal entry channel. However, stem-loop 1 (SL1) in the 5´ UTR of the SARS-CoV-2 genome can be recognized by Nsp1 and selectively facilitates viral translation. Since Nsp1 sequences are highly conserved across different SARS-CoV-2 variants and related viruses, we developed a dual-luciferase assay to discover Nsp1 inhibitors with the potential to exhibit broad-spectrum antiviral activity. We identified P23E02 through in-house library screening, utilizing a luciferase assay in a high-throughput manner. P23E02 specifically disrupts Nsp1–SL1–40 ribosome ternary complex by directly binding with the N-terminal domain of Nsp1. Based on alanine mutagenesis and differential scanning fluorimetry, key residues for binding and inhibitory activity of P23E02 were determined. In addition, immunofluorescence-based assays revealed that P23E02 show antiviral activities against SARS-CoV-2 variants and SARS-CoV replication. Intriguingly, P23E02–remdesivir combination exhibits synergistic interaction with improved activity. Delving into how Nsp1 operates and how P23E02 interferes with its function provides valuable insight into understanding the lifecycle of SARS-CoV-2. P23E02 can be a good starting point to develop novel Nsp1 inhibitors for broad-spectrum antiviral therapeutics.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 09:24

Chair: Jonghoon Kim (Soongsil University)

Unveiling the mechanism of action of reversible, covalent 3R/4R tau aggregation inhibitors through a molecular dynamics approach.

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 oligomerization and aggregation of tau protein is a central event in the pathogenesis of Alzheimer's disease and other tauopathies, thus making directly-acting aggregation inhibitors one of the most promising strategies for the treatment of several neurodegenerative conditions. Among many factors, intermolecular tau disulfide bridges were shown to facilitate aggregation, and the oxidation of tau Cys residues is thought to have a protective effect. Recently, levosimendan was shown to inhibit tau oligomerization and disrupt pre-formed tau fibrils *in vivo*. However the mechanism by which covalently acting agents disaggregate tau fibrils remains unclear.In this work, we investigated potential drug binding sites at the top layers of a many-layer, long AD tau paired-helical fibril and elucidated the binding modes of reversible, covalent tau aggregation inhibitors by using computational methods. A combination of molecular docking and molecular dynamics (MD) simulations was performed. We modeled a 5-layer tau fibril, using molecular restraints to imitate the presence of intermolecular forces present in long tau fibrils. 200 ns long, all-atom MD simulations with and without inhibitor molecules were used to examine the atom group movement at the fibril ends and monitor small molecule binding events. Simulations with added PET tracers were used as controls to represent the case of tau binders lacking fibril-disrupting properties. The simulations uncover a novel binding site adjunct to tau Cys322, and demonstrate contrasting binding modes of binder molecules that lack fibril disrupting ability from that of covalent tau

aggregation inhibitors. Thus we hope to make a first step toward the rational drug design of tau aggregation inhibitors.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 09:36

Chair: Jonghoon Kim (Soongsil University)

Exploration of Tetrahydroisoquinoline- and Benzo[c]azepine-Based Sphingosine 1-Phosphate Receptor 1 Agonists for the Treatment of Multiple Sclerosis

Eun Ji Cha, Jushin Kim, Lizaveta Gotina[1], Jaehwan Kim, Hyeon Jeong Kim, Hak Joong Kim[2], Ae Nim Pae[*], Ki Duk Park[*], Jong-Hyun Park[*], Sang Min Lim[*]

Center for Brain Disorders, Brain Science Institute, Korea Institute of Science and Technology, Korea
[1]*Department of Bio-Medical Science and Technology, University of Science & Technology, Korea*
[2]*Department of Chemistry, Korea University, Korea*

Because of the wide use of Fingolimod for the treatment of multiple sclerosis (MS) and its cardiovascular side effects such as bradycardia, second-generation sphingosine 1-phosphate receptor 1 (S1P1) agonist drugs for MS have been developed and approved by FDA. The issue of bradycardia is still present with the new drugs, however, which necessitates further exploration of S1P1 agonists with improved safety profiles for next-generation MS drugs. Herein, we report a tetrahydroisoquinoline or a benzo[c]azepine core-based S1P1 agonists such as 32 and 60 after systematic examination of hydrophilic groups and cores. We investigated the binding modes of our representative compounds and their molecular interactions with S1P1 employing recent S1P1 cryo-EM structures. Also, favorable ADME properties of our compounds were shown. Furthermore, in vivo efficacy of our compounds was clearly demonstrated with PLC and EAE studies. Also, the preliminary in vitro cardiovascular safety of our compound was verified with human iPSC-derived cardiomyocytes.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 09:48

Chair: Jonghoon Kim (Soongsil University)

Peptide-Nucleic Acid (PNA)-Encoded Chemical Libraries

Jun Hyung Park, Jungyeon Kim, Hyun-Suk Lim*

Department of Chemistry and Division of Advanced Materials Science, Pohang University of Science and Technology, Korea

DNA-encoded libraries (DELs) have proven to be a valuable platform for efficient and streamlined protein ligand discovery. However, in current DEL technology, the chemistry for library synthesis is limited because DNA is insoluble in organic solvents and easily damaged under many reaction conditions, making it highly incompatible with organic reactions. Here, we present peptide-nucleic acid (PNA)-encoded library technology using PNA, a synthetic mimetic of DNA, as an alternative encoding material. In contrast to DEL synthesis, which is performed in aqueous buffer with unprotected nucleobases, PNA-encoded synthesis can be accomplished via solid-phase synthesis with protected bases, thereby making it more compatible with organic reactions. Thus, the reactivity scope and structural diversity of compounds in PNA-encoded library can be largely expanded. The feasibility and utility of the technology was validated by a model selection using streptavidin, and applied to the selection of a PNA-encoded small-molecule library and a peptidomimetic library against carbonic anhydrase IX (CAIX) and glycogen synthase kinase-3 beta (GSK3β), respectively.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Oral Presentation : **MEDI.O-6**
Oral Presentation of Young Medicinal Chemists
Convention Hall 1 THU 10:00
Chair: Jonghoon Kim (Soongsil University)

Discovery of (+)-SHIN2 analogues exhibiting improved SHMT2 activities

Vineetkumar Bapusaheb Patil, **Pilho Kim**[1,*]

Medicinal Chemistry, University of Science & Technology / KRICT, India
[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Cancer cells alter their metabolism to fuel their growth and proliferation in which folate-dependent one-carbon metabolism (OCM) plays a vital role in these processes. Serine hydroxymethyltransferase (SHMT) is a key enzyme in OCM, contributing to the synthesis of essential cellular components crucial for cancer cell survival. SHMT converts serine and tetrahydrofolate (THF) into glycine and 5,10-methylene tetrahydrofolate (Me-THF), respectively, which is elevated in cancer cells. Thus, blocking the function of SHMT can be an effective strategy to starve the cancer cells of their necessary fuel and subsequently reduce the tumor growth. Human SHMT exists in two isoforms, the cytosolic SHMT1 and mitochondrial SHMT2, both carrying out the same function, however, SHMT2 is directly involved in the survival, proliferation, and invasion of various cancers. Genetic deletion of mitochondrial SHMT2 gene reduced the tumor growth in mice, validating SHMT2 as a target for cancer treatment. Several inhibitors have been explored to target SHMT1/2, out of which pyrazolo pyran scaffolds dominate the chemical space. Although (+)-SHIN2 and a THF mimic AGF347 displayed in vivo anti tumor effect in mice, they lack metabolic stability. Due to the lack in metabolic stability, the drug is metabolized quickly in the liver, resulting in the requirement of higher doses to induce pharmacological effects. Hence, new inhibitors with enhanced potency and favorable in vivo pharmacokinetics would help overcome these issues.As our ongoing efforts of anti-cancer drug discovery, we designed and synthesized SHMT2 inhibitors based on SHIN2, and evaluated their activities and druggbilities. In this study, we describe the chemistry and biological evaluation of SHMT2 small molecule inhibitors. During the course of our research, we discovered SHMT2 inhibitors with enhanced activity, which might lead to the discovery of potential anti-cancer agents.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 10:12

Chair: Jonghoon Kim (Soongsil University)

Total synthesis and immunological activities of Bacteroides fragilis α-galactosylceramides and their analogues

Jesang Lee, Sungwhan F. Oh[1,*], Seung Bum Park[*]

Department of Chemistry, Seoul National University, Korea

[1]*Department of Anaesthesia, Brigham and Women's Hospital, United States*

Recently, molecular mechanisms behind the human immunity–microbiota interactions have received growing attention to understand and treat the human diseases. Bacteroides fragilis (B. fragilis) is one of the human gut symbionts which is known to play an important role in homeostasis of human gut immune system. For example, unique α-galactosylceramide (α-GalCer) from B. fragilis has been revealed as a key molecular mediator of human gut immune development at neonatal stage. However, it was difficult to build a library of structurally diverse α-GalCer derivatives from B. fragilis through conventional α-GalCer synthesis. Previously, we have reported a novel synthetic route for efficient late-stage modification of sphinganine and acyl chains of α-GalCer. However, copper-catalyzed cross coupling reaction of sphinganine chain in the presence of triple bonds required an additional step of converting incompatible functional groups and resulted in low yield due to the side reaction. Herein, we have developed a novel synthetic route for sphinganine chain of α-GalCer using Grubbs metathesis. The partner olefin required for metathesis with the sphinganine intermediate could be structurally diversified by copper-catalyzed cross coupling. The in vitro and in vivo immunological assay of B. fragilis α-GalCer library shed new light on the structure–activity relationship of α-GalCer.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 10:24

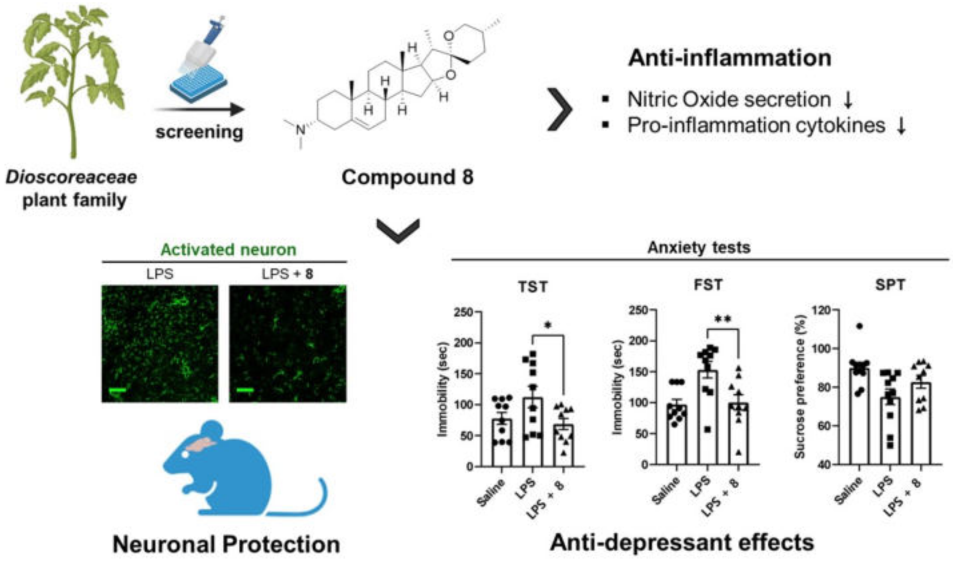
Chair: Jonghoon Kim (Soongsil University)

Neuroprotective effects of diosgenin derivatives with anti-inflammatory effects for antidepressant potential

Younghoon Yoo, Sanghee Lee*, Byungsun Jeon*

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

Depression is a prevalent mental illness affecting approximately 300 million people globally, with its prevalence continuously rising. Drugs such as tricyclic antidepressants and selective serotonin reuptake inhibitors are widely used in clinical practice, however, their notable side effects hinder complete treatment of depression. Hence, there is need to develop novel antidepressants with fewer side effects. Diosgenin, a phytosteroid sapogenin and an active ingredient derived from dioscin found in *Dioscoreaceae* plant family, possesses various pharmacological properties and has a potential for the treatment of neurological disorders. However, diosgenin faces challenges in clinical application due to poor solubility and limited bioavailability. This study aims to develop diosgenin derivatives and to investigate the potential as an antidepressant candidate. Among the diosgenin derivatives, compound 8 stood out the best TI value of 19.8, effectively inhibiting LPS-induced NO production while showing minimal cell toxicity (IC_{50}: 667.5 μM). Further investigations revealed that compound 8 effectively suppressed neuroinflammation in microglia cells by monitoring inflammatory markers. In a co-culture study involving BV-2 cells and HT22 neuronal cells, compound 8 demonstrated neuroprotective property. Moreover, compound 8 could ameliorate LPS-induced reactive astrogliosis and microgliosis in the hypothalamus. We further evaluated *in vivo* efficacy of compound 8 using three different behavioral tests with ICR mice, resulting in recovery of LPS-induced depressive phenotype, particularly despair behaviors. We demonstrated that compound 8 exhibited neuroprotective property without cytotoxicity and suppressed neuroinflammation especially in hypothalamus. Our findings further suggest that compound 8 has therapeutic potential as new type of antidepressant.


Dioscoreaceae plant family
screening
Compound 8
Anti-inflammation
Nitric Oxide secretion ↓
Pro-inflammation cytokines ↓
Activated neuron
LPS
LPS + 8
Neuronal Protection
Anxiety tests
TST
FST
SPT
Immobility (sec)
Sucrose preference (%)
Saline
LPS
LPS + 8
*
**
Anti-depressant effects

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 10:36

Chair: Jonghoon Kim (Soongsil University)

Design and Development of Anaplastic Lymphoma Kinase (ALK) Degrader via Covalent Fumarate Handle

Namsik Yu, Jong Yeon Hwang[1,*]

Department of chemistry, Sungkyunkwan University, Korea

[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Recently, the concept of targeted protein degradation, including methods like Proteolysis Targeting Chimera (PROTAC) and molecular glue, has generated significant interest in the field of drug discovery as an innovative therapeutic approach. In our endeavors to degrade the anaplastic lymphoma kinase (ALK), we harnessed FDA-approved drugs like crizotinib, ceritinib, brigatinib, and alectinib, utilizing them as binders for ALK, alongside 4-methoxyphenylfumarate as a covalent handle to bind with for RNF126 E3 ligase. Among the synthesized compounds, particularly one known as dALK-3, derived from brigatinib, displayed a remarkable ability to induce the proteasomal degradation of EML4-ALK in a dose-dependent manner. We tested this in H3122, a non-small-cell lung cancer cell line known to carry the oncogenic EML4-ALK fusion protein. Remarkably, dALK-3 exhibited an approximately 10-fold superior anti-proliferative effect on H3122 cells compared to brigatinib, despite having a weaker inhibitory effect on ALK. These findings strongly indicate that the exceptional anti-proliferation impact of dALK-3 can be attributed to ALK degradation rather than its catalytic inhibition. Furthermore, it's noteworthy that our experiments, involving the depletion of RNF126 through specific siRNA, revealed that the anti-proliferative effect of dALK-3 is independent of RNF126. This raises the possibility that other components within the ubiquitin-proteasome system (UPS) may be involved in this observed effect. Consequently, further investigations are crucial to identify the specific E3 ligase responsible for this effect.

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

Oral Presentation of Young Medicinal Chemists

Convention Hall 1 THU 10:48

Chair: Jonghoon Kim (Soongsil University)

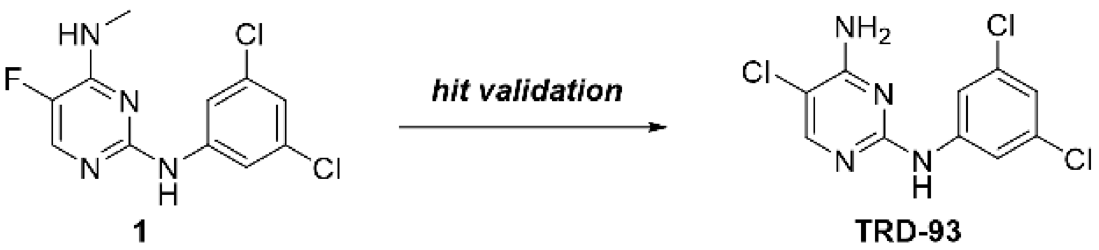
Identification of TRD-93 as a novel DRAK2 inhibitor

Kwangho Lee*, Seungmin Kye[1]

Korea Research Institute of Chemical Technology, Korea

[1] *University of Science & Technology, Korea*

Death-associated protein kinase-related apoptosis-inducing protein kinase 2 (DRAK2), also known as serine/threonine kinase 17B (STK17B), belongs to the family of death associated protein kinases (DAPKs) along with DAPK1, DAPK2, DAPK3, and DRAK1. DRAK2 expression is highly elevated in multiple tumor types such as basal-like and HER2-enriched breast cancers: knockdown of the DRAK2 gene results in significant tumor growth inhibition in a mouse xenograft animal model. Therefore, DRAK2 has emerged as a promising drug target for the treatment of cancers. However, only a small number of DRAK2 inhibitors have been reported so far but many of them lack drug-likeness.In search of novel and selective DRAK2 inhibitor motif, *in vitro* screen kinase assay was established and performed using in-house chemical libraries. After through hit triage procedure, N^2-(3,5-dichlorophenyl)-5-fluoro-N^4-methylpyrimidine-2,4-diamine (1) was selected as a initial hit with structural novelty and drug-likeness. During hit validation, SAR of 1 was disclosed and TRD-93 was finally validated as a hit for DRAK2 inhibition. In this oral presentation, we report TRD-93 is potent and selective DRAK2 inhibitor (IC_{50} = 0.16 μM) and its molecular binding mode.


1
hit validation
TRD-93

Oral Presentation : **MAT.O-1**
Oral Presentation for Young Material Chemists
Room 201+202+203 THU 09:00
Chair: Jiwoong Yang (DGIST)

Narrow bandgap infrared sensitive colloidal quantum dots and optoelectronic applications

Dongsun Choi, Gahyeon Kim[1], Jin Hyeok Lee[1], So Young Eom, Kwang Seob Jeong*

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

Infrared optoelectronic applications have attracted much attention due to high interest from healthcare, medical devices, automatic transportation sensors, and defense. Common infrared optoelectronic applications in the past few decades have mainly developed based on epitaxial toxic materials, necessitating high-cost equipment and material hazards during fabrication. To overcome these limitations, non-toxic CQDs are considered alternative materials for future optoelectronics. Here, we represent infrared sensitive narrow bandgap materials and optoelectronic application results, fulfilling the prerequisite requirements in various fields. Silver telluride (Ag2Te) CQDs have extended the infrared photodiode region to eSWIR, reaching the highest 16 % of external quantum efficiency (EQE). Surprisingly, the colloidal ink state of Ag2Te CQDs is fabricated under ambient conditions, allowing homojunction device fabrication, which increases the cost-effectiveness of the infrared CQDs. Indium antimonide (InSb) CQDs are successfully synthesized using zinc halide and remarkably reaching ~75 % EQE at 1250 nm, showing the highest EQE among the indium system.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 09:10

Chair: Jiwoong Yang (DGIST)

Understanding Mechanism of Mechanoluminescence in ZnS:Cu Microparticle Embedded Polydimethylsiloxane Composites: Electroluminescence Induced by Interfacial Triboelectricity

Gyudong Lee, Sung Jun Lim*

Division of Nanotechnology, Daegu Gyeongbuk Institute of Science & Technology, Korea

Since its first report in 2013, Cu-doped ZnS microparticle embedded in polydimethylsiloxane (ZnS:Cu-PDMS) composite has attracted considerable attention due to its bright and durable mechanoluminescence (ML). This unique material distinguishes itself from previously reported ML materials, which typically exhibit low and unrepeatable ML characteristics. Over the past decade, a wide range of ML applications have been demonstrated using ZnS:Cu-PDMS composites such like full-color ML displays, self-powered ML fabrics, motion sensor. However, the mechanism underlying the distinctive ML characteristics observed ZnS:Cu-PDMS composite has not been remains unclear, posing a significant obstacle to related research and development efforts. In this study, we present empirical and theoretical findings to elucidate the bright and repeatable ML observed in the ZnS:Cu-PDMS composite, which is an electroluminescence (EL) phenomenon originating from the ZnS:Cu microparticles due to triboelectricity generated at the ZnS:Cu microparticle-PDMS interface. Our investigation reveals that friction between the surface of ZnS:Cu microparticles coated with alumina, an oxide with strong positive triboelectric properties, and PDMS, a strong negative triboelectric properties, generates sufficient interfacial triboelectricity to activate the EL of ZnS:Cu microparticles. With this finding, we conducted change the composition of interface and demonstrated close correlation between ML intensity and interfacial triboelectricity. Also, surface charge density calculations provide further support for our proposed model. Understanding such a mechanism will play a crucial role in exploring and advancing

new materials beyond the ZnS:Cu-PDMS systems to achieve brighter and more durable ML composite systems.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 09:20

Chair: Jiwoong Yang (DGIST)

New defect structure design for exceptional thermoelectric performance in new n-type $Cu_xPb(Se_{0.8}Te_{0.2})_{0.95}$ ($x = 0 – 0.0057$) compounds

Hyungseok Lee, **Bangzhi Ge**[1], **Chung In**[2,*]

Institute of Chemical Processes, Seoul National University, Korea

[1]*State Key Laboratory of Solidification Processing & Key Laboratory of Radiation Detection Materials and Devices, Northwestern Polytechnical University, China*

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

Every material has an imperfect crystal lattice extrinsically by doping and alloying as well as intrinsically, consequently forming local structures at the atomic-level. They may interact and extend to construct more complex defects, and significantly affect bulk properties of materials. However, directly observing such defect structures and investigating their direct influences on bulk properties have been critically less studied. In this talk, I present the stabilization of complex defect architectures consisting of interstitial Cu, Pb and Se atoms off-centered from the ideal crystallographic sites, dislocation initiated by anion vacancies, and multidimensional nanostructures by in the new compounds $Cu_xPb(Se_{0.8}Te_{0.2})_{0.95}$ ($x = 0 –$ 0.0057). The results of direct observation for the defect structures using an atomic-resolution Cs-corrected STEM will be discussed. The best composition snows surprisingly high average power factor ~24 μW cm^{-1} K^{-2} from 300 to 823 K, and record high achieved average thermoelectric figure of merit, ZT, is ~1.3 from 400 to 823 K, for all n-type PbSe and PbTe-based materials to date.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 09:30

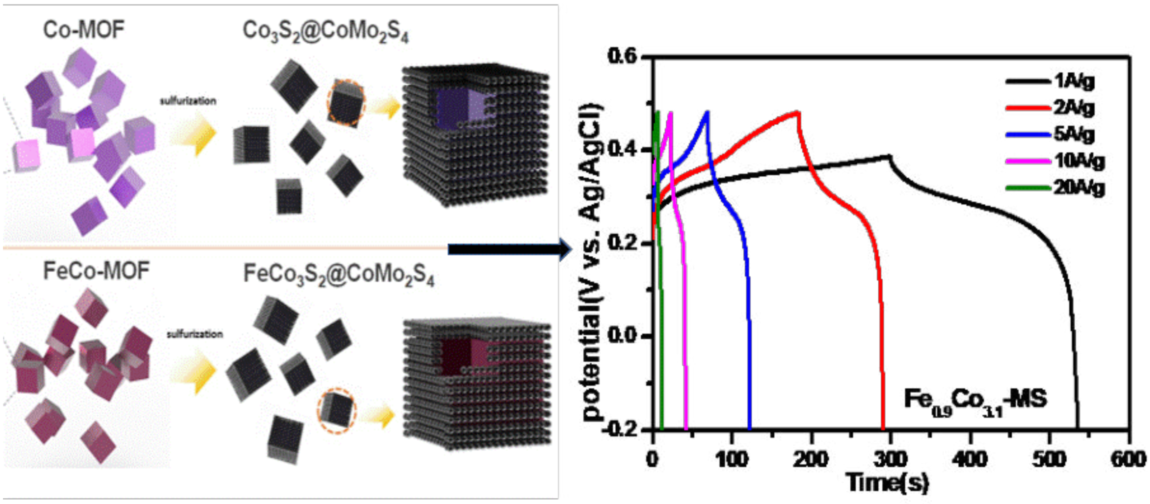
Chair: Jiwoong Yang (DGIST)

Attempts to unlock the puzzle box in Low-cost advanced electrode materials for energy storage application.

Njemuwa Nwaji Njoku

Chemistry, Chungnam National University, Korea

Vacancy engineering offers an attractive approach to improve the surface properties and electronic structure of transition metal nanomaterials. However, simple and cost-effective methods for introducing defects into nanomaterials still face great challenges. Herein, we propose a facile room temperature two-step technique that utilizes Fe as dopants to enhance S vacancies in cobalt-based metal−organic frameworks (MOFs). The Fe-Co-MOF was converted into a hollow Fe-Co3S4 confined in CoMo2S4 to form Fe-Co3S4@CoMo2S4 nanosheets. The as-prepared material showed enhanced charge storage kinetics and excellent properties as electrode material for supercapacitors. The obtained nanostructure displayed a high specific capacitance (980.3 F g-1 at 1 A g−1) and excellent cycling stability (capacity retention of 87.5% after 6,000 cycles at 10 A g−1). Density functional theory (DFT) calculations show that introducing defects into the nanostructures leads to more electrons appearing near the Fermi level, which is beneficial for electron transfer during electrochemical processes. Thus, this work provides a rational cost-effective strategy for introducing defects into transition metal sulfides and may serve as a potential means to prepare electrode materials for energy storage.


Co-MOF
sulfurization
Co_3S_2@$CoMo_2S_4$
FeCo-MOF
sulfurization
$FeCo_3S_2$@$CoMo_2S_4$
potential(V vs. Ag/AgCl)
Time(s)
0.6
0.4
0.2
0.0
-0.2
0
100
200
300
400
500
600
1A/g
2A/g
5A/g
10A/g
20A/g
$Fe_{0.9}Co_{3.1}$-MS

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 09:40

Chair: Jiwoong Yang (DGIST)

Multifunctional phosphine oxide derivatives for CsPbBr3 emissive layer with high efficiency

Jung Min Ha, Han Young Woo*

Department of Chemistry, Korea University, Korea

Perovskite light-emitting diodes (PeLEDs) are garnering significant attention as promising candidates for the next-generation display technology due to their narrow bandwidth, high external quantum efficiency (EQE), and luminance. The optical and photoelectrical properties of perovskite are strongly influenced by its crystallinity, crystal size, and defects density, which give rise to trap states responsible for non-radiative recombination, thereby limiting EQEs in devices. This study specifically focuses on the utilization of covalently bond triphenylphosphine oxides (TPPO) molecules within the 3D nanostructured CsPbBr3 perovskite emissive layer. The multifunctional TPPO derivatives effectively passivate surface defects by forming robust bonds with PbBr2. Importantly, their presence delays the binding of bromide with PbBr2 due to significant steric hindrance when incorporated into the perovskite precursor solution. This, in turn, facilitates the formation of perovskite films with smaller grain sizes and enhanced quantum efficiency of resulted PeLED.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Oral Presentation : **MAT.O-6**
Oral Presentation for Young Material Chemists
Room 201+202+203 THU 09:50
Chair: Jiwoong Yang (DGIST)

Precursor stoichiometry control enabling of $CsPb(Cl/Br)_3$ blue quantum dots synthesis via one-pot design

Jin Young Kim, Dong Hwan Wang*

College of ICT Engineering School of Integrative Engineering, Chung-Ang University, Korea

Perovskite-based blue-emitting colloidal particles are useful for a number of applications by applying the multi-exciton generation and superior properties of their composed materials. However, cesium-based blue perovskite quantum dots (PQDs) have low stability due to the use of two halogen materials, and are difficult to manufacture due to a complicated process. We would like to propose a method that can overcome the complex manufacturing process and synthesize blue PQDs in the ambient environment. We minimized by-products generated during the synthesis process and confirmed the optical stability of blue light emission. As a result, we synthesized $CsPbClBr_2$ BQDs with a quantum yield of 70.55% and FWHM of 14 nm. It was confirmed that the optical properties were maintained for 400 hours without discoloration due to the aggregation of the $CsPbClBr_2$ QDs. In addition, it confirmed the stability of the perovskite structure by preparing a double layer of deionized water and re-dispersion solvent. These results suggest a one-pot design to produce high-purity $CsPbClBr_2$ in an ambient environment.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 10:10

Chair: Jiwoong Yang (DGIST)

Exfoliated noble-metal-free conductive oxide nanosheets as efficient hybridization matrix

Namhee Kwon, Xiaoyan Jin, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

Hybridization with conductive 2D nanosheets has evoked intense research activities because of their effectiveness for optimizing the photocatalyst performance of diverse semiconductors. To circumvent the high price and limited electronic coupling of previously-reported graphene and/or RuO_2 nanosheets, here we suggest the synthesis of economically-feasible noble-metal-free conductive nanosheets via the fine-control of chemical composition and defect structure. The diversification of cationic composition of multimetallic oxide nanosheet enables to finely tailor anion vacancy and surface bond polarity, leading to a strong interfacial electronic coupling with hybridized species and thus an improvement of charge/mass transfer. The composition-optimized multimetallic oxide nanosheets can function as superior hybridization matrices for enhancing visible light ($\lambda > 420$ nm) photocatalytic activities over graphene and noble metal-based RuO_2 nanosheet. The present study highlights the high efficiency of composition-controlled multimetallic oxide nanosheets as hybridization matrices for photocatalysts.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 10:20

Chair: Jiwoong Yang (DGIST)

Insights into the Formation and Behavior of Graphene Oxide Langmuir-Blodgett films at the Air-Water Interface

Jae-Joon Lee[*], Sang Jung Ahn[1,*], Jongdeok Park

Department of Energy and Materials Engineering, Dongguk University, Korea

[1]*Center for Advanced Instrumentation, Korea Research Institute of Standards and Science, Korea*

The π-A isotherm obtained during the formation of Langmuir-Blodgett (LB) films of various nanomaterials offers comprehensive information into the behavior of nanomaterials and the bulk phase of LB films at the air-water interface. Therefore, the behavior of the material and the bulk phase of the LB film could be predicted by the surface pressure and compressional modulus without the process of transferring and analyzing the LB film. However, predicting the bulk phase of the LB film using surface pressure and compressive elastic modulus proved difficult, as soft-2D nanomaterials such as graphene oxide undergo deformation during compression. Therefore, to confirm the bulk phase of the GO LB film, the transfer and optical analysis of the LB film was required. In this study, we proposed a new approach to predict the bulk phase of GO LB films at the air-water interface without transfer and analysis using dynamic dilatational modulus. Furthermore, the surface structure of the GO LB film is effectively controlled by adjusting the size distribution of GO in the solution. The wrinkled-rGO LB film exhibits higher catalytic activity than the overlapped-rGO LB film based on the large surface area. In the future, our research is expected to be applicable to soft 2D nanomaterials as well as graphene oxide, offering deeper insight into thin film formation.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 10:30

Chair: Jiwoong Yang (DGIST)

Synthesis of a Surfactant-Free Mixed-Valence Rhenium Oxide Nanocubes and their Photocatalytic performance

Kang min Lee, **Seok Min Yoon**[1,*]

Department of chemistry, Wonkwang University, Korea

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

Surfactant-free mixed-valence ReO_3 nanocubes (MVReO_3-SF-NCs) were successfully synthesized via a wet-chemical method without surfactant. The as-synthesized MVReO_3-SF-NCs show an overall broad absorption spectrum from near UV to NIR. When MVReO_3-SF-NCs were photodegradation placed in methyl orange aqueous solution under artificial sunlight (> 400 nm), the results demonstrated that degraded enhance than surfactant-anchored mixed-valence ReO_3 nanoparticles (MVReO_3 SA-NPs) and TiO_2 (P25). Furthermore, MVReO_3-SF-NCs were placed in Rhodamine B aqueous solution for photodegradation by irradiation artificial sunlight (> 400 nm), the results that their performed better than MVReO_3-SA-NPs and TiO_2 (P25). The results suggest that the surface of the cleaned photocatalyst, the different mixed-valence oxidation states, and the localized surface plasmon resonance (LSPR) are key to improving the photocatalytic efficiency and that the improved MVReO_3-SF-NCs have potential applications not only in dye photodegradation, but also in water splitting, CO_2 conversion, environmental remediation, and solar cells.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 10:40

Chair: Jiwoong Yang (DGIST)

Porous microstructure coated by whitlockite nanocrystals for bone restoration

Hyojin Kang, Caifeng Wang[1], Jaebeom Lee[2,*]

Chemical engineering and Applied chemistry, Chungnam National University, Korea

[1]*CAS Key Laboratory for Biomedical Effects of Nanomaterials and Nanosafety, National Center for Nanoscience and Technology of China, China*

[2]*Chemistry, Chungnam National University, Korea*

Whitlockite (WH; Ca18Mg2(HPO4)2(PO4)12), the second most abundant bone mineral, is gaining attention as a novel substance for bone regeneration. It is abundant in areas of the actual human bone that bear weight and is present in a high proportion in juvenile bone tissue. As individuals age, it gradually diminishes, playing a significant role in the early stages of bone formation. In this study, to enhance bone regeneration through whitlockite, a bone graft was fabricated by coating whitlockite onto the surface of hydroxyapatite porous microstructures. The coated nanoparticles were synthesized in high purity on a 1L scale, and their quality was assessed using analytical techniques such as TEM, SEM, and XRD. Additionally, the produced bone microstructures exhibited a remarkable capability to promote bone regeneration in the Invitro experiment. Furthermore, upon transplantation into bone defects in rats, these engineered microstructures exhibited exceptional regenerative capacity, particularly when combined with BMP. This study underscores the promise of whitlockite-coated grafts as a powerful tool in advancing bone tissue regeneration, offering substantial potential for clinical applications and further research.

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

Oral Presentation for Young Material Chemists

Room 201+202+203 THU 10:50

Chair: Jiwoong Yang (DGIST)

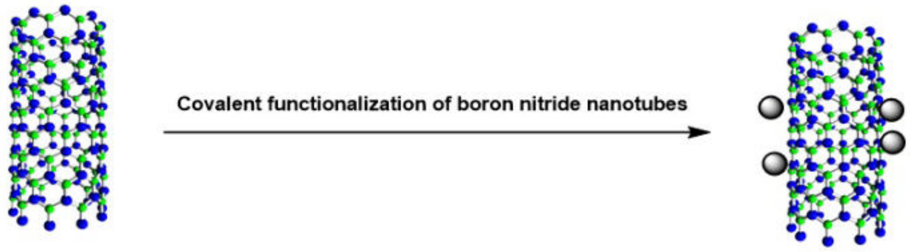
Covalent Functionalization of Boron Nitride Nanotubes via Coupling Reaction

Thang Quoc Huynh, **Seokhoon Ahn**[1,*]

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

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

Boron nitride nanotubes (BNNTs) have captivated attention as an inorganic counterpart to carbon nanotubes (CNTs), possessing unique properties such as electrical isolation, exceptional thermal stability, and neutron-blocking capabilities. However, BNNTs are usually found in aggregates held together by weak van der Waals forces, leading to low dispersion in organic solvents, which limits their applications. To overcome this challenge, a promising approach involving covalent functionalization has been proposed, utilizing benzene diazonium tetrafluoroborate and its derivatives to graft organic components onto the BNNT surface. Extensive analysis of chemical structure, composition, and morphology provided compelling evidence of successful functionalization. Thermogravimetric characterization confirmed significant weight loss (up to 21.8%), validating the grafting of organic components onto BNNTs. Moreover, dispersion tests demonstrated the stabilization of functionalized BNNTs in solvents for extended periods, showcasing the potential to enhance their processability and reactivity for a wider range of applications



Previous reports

x harsh acids to oxidize the B–N bond
x relying on more elegant or exotic reduction techniques
x multi steps reaction, harsh condition
x low degree of functionalization

Our report

✓ no strong acids, potent oxidazing agents
✓ no metallic materials
✓ facile synthesis, 1 step reaction
✓ preserve nanotube structure
✓ high degree of functionalizations
✓ broad scope

Award Lecture in Division : **ELEC.O-14**

Oral Presentation for Young Electrochemists

Room 206+207 THU 10:31

Chair: Jun Hui Park (Chungbuk National University)

Redox reversibility controls of redox active organic molecules for aqueous energy storage systems

Jinho Chang

Department of Chemistry, Hanyang University, Korea

Enhancing redox reversibility of redox active organic molecules is important in various aqueous energy storage systems (e.g. electrochemical capacitor and redox flow battery). The two different approaches for redox reversibility enhancement are presented in this talk. At first, we fully demonstrated that ascorbic acid (ASC), which is an abundant but redox-irreversible molecule, can become redox-reversible when it is confined in microporous carbon regimes. The origin of nanoporous confinement of ASC and its enhanced redox-reversibility was rationalized by molecular dynamics simulations. We found that ASC-clusters of a fully protonated ASC and its conjugated base formed inside carbon pores, which would be a main driving force for its confinement in microporous carbon networks. Lastly, we demonstrated a prototype energy storage device using redox-reversible ASC in microporous carbon as the half electrode, which shows the feasibility of ASC as a possible redox electrolyte in an aqueous energy storage system. In the second, we show that a covalent conjugation of a 'hydroxide-philic' functional group to TEMPO moiety is the key to effectively mitigating chemical degradation during charging and discharging, which hinders OH^--access to oxoammonium sites in the intramolecular regime, leading to a stable TEMPO-based aqueous organic redox flow battery (AORFB) with long-term cyclability.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:00

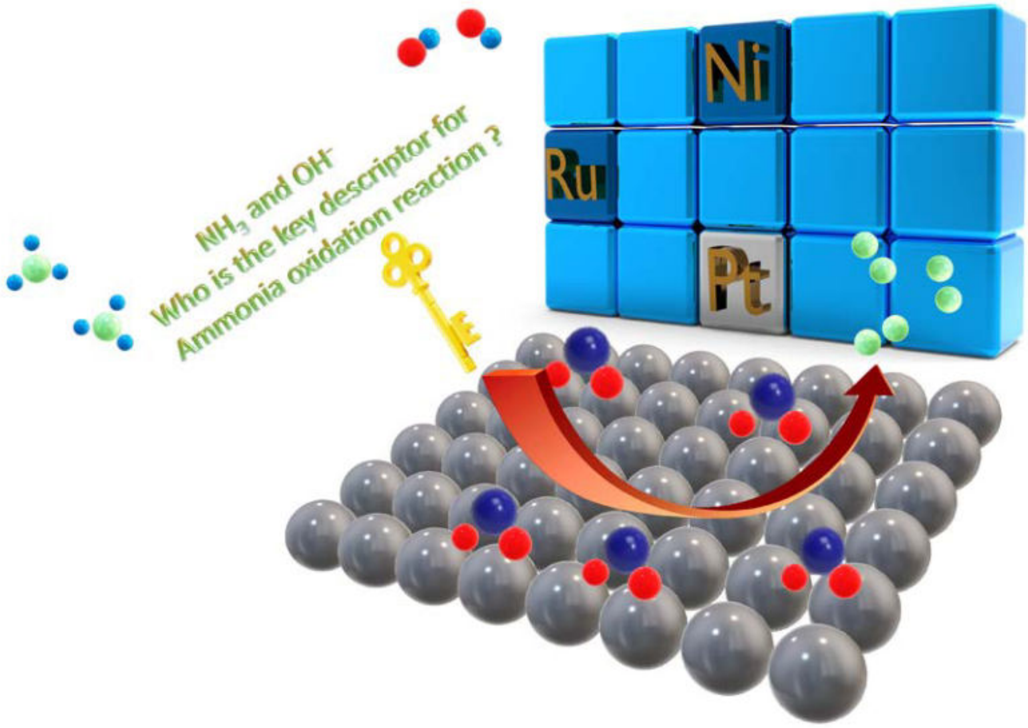
Chair: Changsuk Yun (Changwon National University)

NH_3-philicity Modulation via Atomic Metal Decorated Pt Nanocube Tracing the Ammonia Oxidation Reaction Descriptor

Jungki Kim, Juhyun Cho, Jeonghyeon Kim, Saehyun Park[1], Shajahan Shaik[1], Sang-Il Choi[*]

Department of Chemistry, Kyungpook National University, Korea
[1]*Department of Chemisty, Kyungpook National University, Korea*

The impact of NH_3 and OH adsorption on AOR activity is uncertain. To address this, we synthesized $Ni_{at}Pt$ NCs/C and $Ru_{at}Pt$ NCs/C catalysts with Ni and Ru as single-atom sites on platinum cubes, exhibiting strong oxophilicity. Both catalysts showed enhanced OH adsorption, and only $Ni_{at}Pt$ NCs/C had increased NH_3 adsorption. AOR activity was 1.14 and 0.83 times higher for $Ni_{at}Pt$ NCs/C and $Ru_{at}Pt$ NCs/C, respectively, compared to Pt NCs/C. This suggests NH_3 adsorption plays a more direct role in AOR activity than OH adsorption, making it the key descriptorThis work was financially supported by the k-water Project Open Innovation R&D (OSK_2022_036)


NH3 and OH-
Who is the key descriptor for
Ammonia oxidation reaction ?
Ni
Ru
Pt

Oral Presentation : **ELEC.O-2**
Oral Presentation for Young Electrochemists
Room 206+207 THU 09:07
Chair: Changsuk Yun (Changwon National University)

Exceptionally Stable β-NiOOH-Enclosed Fe Doped-Ni Nanoplates for High-Performance Anion Exchange Membrane Water Electrolysis

Jeonghyeon Kim, Sang-Il Choi[1,*]

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

Hydrogen is considered an alternative energy source that can replace fossil fuels and mitigate carbon emissions. Anion exchange membrane water electrolyzers (AEMWEs) have demonstrated the potential to achieve low-cost, high-performance water electrolysis and produce high-purity hydrogen. However, to improve the AEMWE performance, a highly stable and active nanocatalyst is required for the anodic oxygen evolution reaction (OER), which is the bottleneck of the overall electrolysis process. The Ni oxyhydroxides (β-NiOOH) grown on Ni{111} surface have shown promising activity and stability toward OER in alkaline media. To achieve even greater OER stability performance, Fe-doped Ni nanoplates encapsulated by β-NiOOH (FeNi⊥β-OOH NPs) been developed. OER stability test showed that, these nanoparticles maintained a constant current density of 10 mA cm^{-2} for a record-breaking 120 days. AEMWEs fabricated with FeNi⊥β-OOH NPs/C using the catalyst-coated substrate method exhibited a current density of 2256 mA cm^{-2} at 1.8 V with an energetic efficiency of 76.0%. In addition, cell stability test exhibited stable performance at 500 mA/cm^{2} over 500 hr. This remarkable achievement not only demonstrates the potential of FeNi⊥β-OOH NPs in AEMWEs but also opens up new avenues for low-cost, high-performance water electrolysis and hydrogen production. This research has been performed as Project Open Innovation R&D(OTSK_2022_036) and supported by K-water

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:14

Chair: Changsuk Yun (Changwon National University)

Electrochemical Assessment of Polymer Stability: Probing Depolymerization in Cutting-edge Engineering Polymers

Jee Woo Kim, Byung-Kwon Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Polymers' depolymerization control is critical for their application, with molecular weight affecting mechanical properties and processability. Existing evaluation methods like viscosity measures, gel permeation chromatography (GPC), and nuclear magnetic resonance (NMR) spectroscopy have limitations—demanding large samples, lengthy analyses, and missing post-polymerization degradation. To overcome these, we introduce an innovative electrochemical approach based on cyclic voltammetry, enabling real-time tracking of depolymerization during synthesis. This technique leverages the relationship between molecular weight reduction, viscosity decrease, and amplified steady-state current, allowing for a swift and precise assessment of molecular weight changes. The method offers quick measurements, requires small sample sizes, and holds promise for industries reliant on accurate polymer property analysis.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:21

Chair: Changsuk Yun (Changwon National University)

Aerosol derived carbon dots decorated boron nitride supported Zn-doped MoS2 for high performing flexible asymmetric supercapacitor

Chandan kumar Maity, Myung Jong Kim*

Department of Chemistry, Gachon University Global Campus, Korea

Alternative finding of toxic pollutant materials in proper utilization is a great challenge. Toxic and pollutant cigarette smoke having different π-conjugated organic components may work well as a precursor for carbon dots (CDs). In this work, cigarette smoke aerosol has been used for the synthesis of CDs and CDs have been further used for the fabrication of supercapacitor electrode. This methodology could be able to mitigate the two major problems- energy crisis and environment pollution. The smart combination of EDLC-type CDs deposited boron nitride (BN) and pseudocapacitive type Zn-doped MoS2 was able to enhance the supercapacitive performances. Heteroatom doping into MoS2 enhances the capacitive performances through the effective Faradic reactions. CDs and CDs deposited BN (CDs@BN) have been characterized using different characterization techniques. Zn-doped MoS2 has been uniformly grown on the CDs decorated BN (Zn-MoS2/CDs@BN) resulting in the stabilization of the electrode system. Zn-MoS2/CDs@BN nanohybrid delivered a specific capacitance (Sp.C) of 397 F/g in three-electrode system. Further, the asymmetric supercapacitor (ASC) device using Zn-MoS2/CDs@BN as cathode demonstrated wide potential range (up to 1.8 V) with a volumetric energy density of 3.42 mW h/cm3 and retaining a capacitance of ~89% after 10000 charging-discharging processes. Moreover, a flexible ASC device was made-up using viscous ionic electrolyte and it was able to glow a red LED, while it was bended in different angles. The methods described here will give a straightforward approach for using toxic-pollutant cigarette smoke to fabricate supercapacitor electrodes in order to compensate the upcoming energy crisis in a sustainable way.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:28

Chair: Changsuk Yun (Changwon National University)

Pore Opening Effect of Cu-exchanged Zeolites on Electrocatalytic CO_2 and CO Reduction to Multi-carbon Products

Dohun Kim, Dae-Hyun Nam[*]

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

With the crisis of energy deficiency and global climate issues, electrochemical energy conversion systems were considered promising green-energy technology. The electrocatalytic CO_2/CO reduction to multi-carbon products has been spotlighted as the route to attain net-zero emission value-added chemical production. Unfortunately, high-rate CO_2/CO reduction to multi-carbon products was constrained by CO_2/CO mass transport limitation and competition reaction of hydrogen production in high current regions.Herein, we proposed various-type of Cu-exchanged zeolite frameworks for enhancing CO_2/CO mass transport. Zeolite A has a smaller pore opening compared to zeolite X and Y, which can modulate the diffusivity of CO_2 and enhance the local CO_2 concentration. Also, Cu-exchange sites could be manipulated by zeolite types, which increases in the order zeolite A, X, and Y. For these reasons, Cu-Zeolite A exhibited the highest rate of multi-carbon production among the Cu-zeolites. In contrast, CO molecules easily transport through all zeolite frameworks resulting that larger pore sizes achieving more CO concentrations. Therefore, Cu-zeolite X showed a high CO to multi-carbon production performance compared to Cu-zeolite A. X-ray diffraction (XRD) results showed that zeolite frameworks retain their crystal structures after electrocatalytic reactions. Our research demonstrates the potential of extremely stable zeolite-based electrocatalysts to enhance CO_2/CO mass transport for high-rate CO_2/CO conversion to multi-carbon products and opens avenues for their application in diverse electrocatalytic energy conversion systems.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:35

Chair: Changsuk Yun (Changwon National University)

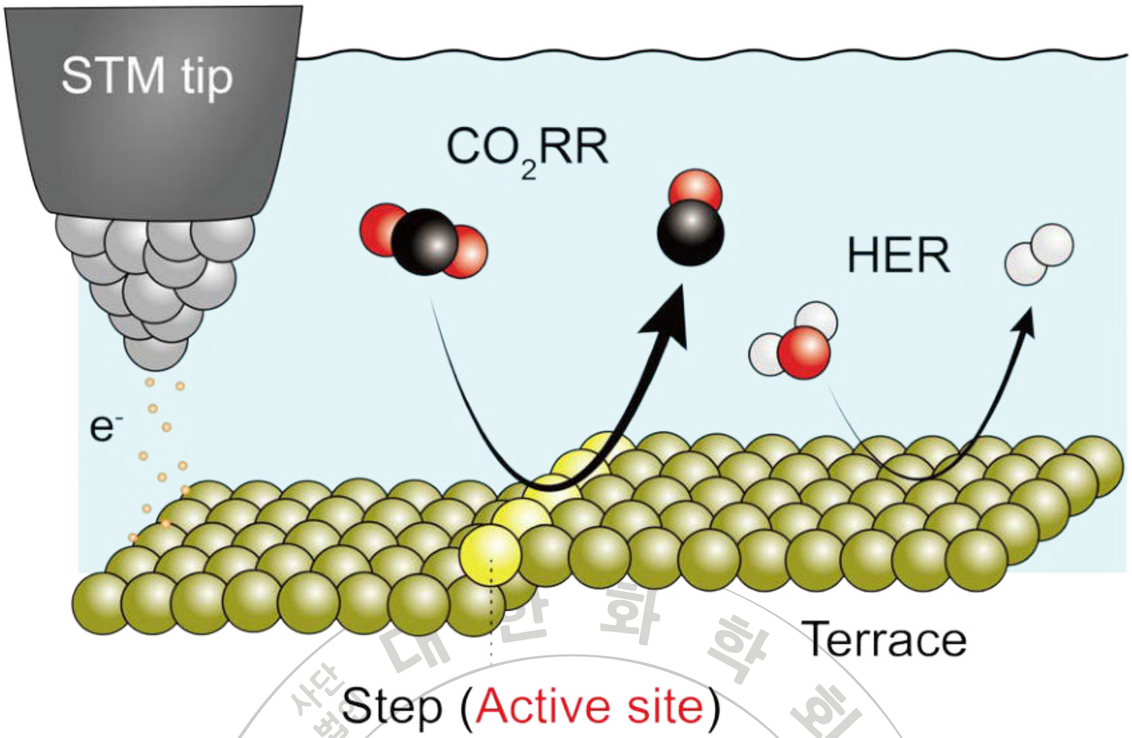
Electrochemical Scanning Tunneling Microscopy Studies of CO_2 Electrocatalytic Reactions on Au(332) Stepped Surface

Yongman Kim, Jeong Young Park[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Independent control of the structure sensitivity of CO_2 electrochemical reduction (CO_2RR) is still challenging due to the intertwined effects of intrinsic factors such as grain boundaries, low-coordinated sites, and oxide species. Furthermore, the atomistic knowledge of the active sites remains elusive, impeded by the intricate relationship between structural stability and catalytic activity. Thus, a fundamental model study is imperative to bridge these materials gap to establish structure-activity relationships in CO_2 electrocatalysis. In this context, we focus on CO production and reaction mechanisms as a key intermediate in CO_2RR. Specifically, we explore the surface structural sensitivity of Au(hkl) single crystals, which serve as a promising candidate in CO production and an ideal system for electrocatalytic CO_2 reduction. Au(hkl) single crystals intuitively show structural dependencies on coordinated sites, including the terrace of the (111) facet and the steps of the (332) facet corresponding to the high-energy facet. CO_2 preferentially reacts with the low-coordinated step (edge) sites and actively converts into CO molecules on the Au(332) surface. Although the stepped Au(332) surface undergoes surface reconstruction under operating conditions, it retains notably higher catalytic activity than the Au(111) surface, underlining the catalytic importance of these low-coordinated step sites.This study establishes a direct relationship between structural changes and catalytic activity, thus providing valuable and unprecedented insights into the proposed mechanism underlying CO_2RR, allowing the enhanced catalyst design and the optimization of sustainable energy conversion processes.


STM tip
CO_2RR
HER
e^-
Terrace
Step (Active site)

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Oral Presentation : **ELEC.O-7**
Oral Presentation for Young Electrochemists
Room 206+207 THU 09:42
Chair: Changsuk Yun (Changwon National University)

Recent progress on transition metal based nanostructures for energy conversion and storage

Goddati Mahendra, Jaebeom Lee[1,*]

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

This article gives an exhaustive assessment of current research focusing on transition metal-based nanostructures (TMNs) for energy conversion and storage. Global energy transformation based on renewable energy sources is pivotal in limiting climate change and achieving sustainable growth. However, the practical use of renewable energy sources craves energy conversion and storage technologies that can improve the sources' efficiency, performance, and density on demand. Clean hydrogen produced sustainably has been touted as a key to decarbonizing global energy systems. Hydrogen, as a potential energy carrier, can serve as a conduit for storing large amounts of energy produced from solar, wind, and other renewable energy sources. Among the many ways, photoelectrochemical water splitting is a promising technology to produce hydrogen sustainably. On the other hand, intermittent renewable energy sources affect their stability, reliability, and power quality. Introducing energy storage systems can be a viable option to address these challenges. Supercapacitors have aroused much interest among different energy storage systems due to their superior power density and long cycle life. Despite progress, these technologies are still at the early age of commercialization, limiting their potential contributions towards carbon-free energy systems. The design of highly efficient, inexpensive, and versatile materials is desired to overcome these limitations. Thus far, high-performing electrocatalysts for electrochemical water electrolysis are based on expensive and scarce noble metals such as Pt, IrO2, and RuO2, restraining the achievement of global scalability. This research covers

fundamental studies of transition metal based TMNs (Fe, Co, Ni, Cu, Zn, Mo, and W) and their design strategies for energy storage and conversion applications. These results indicate advancements towards applications of transition metal based TMNs as an efficient and low-cost material for energy conversion and storage systems.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:49

Chair: Changsuk Yun (Changwon National University)

Investigation of Cation Effects and Mechanisms Governing Electrochemical CO2 Reduction and Hydrogen Evolution in Acidic Media

Hyewon Yun, Suhwan Yoo[1], Yun Jeong Hwang[2,*]

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

Utilizing electrocatalysis for CO2 conversion presents an opportunity to achieve carbon-neutral utilization of carbon-derived chemical resources through renewable energy sources. In the last decade, most electrochemical CO2 reduction reactions (CO2RR) have opted for alkaline and neutral conditions to hinder the competing hydrogen evolution reaction (HER). Nevertheless, the hydroxide ions (OH-) produced during CO2RR and HER react with CO2 to create carbonate, capping the efficiency of CO2 utilization for CO production at 50% or lower. Consequently, conducting CO2RR in an acidic milieu substantially curbs carbon loss and enhances conductivity, thereby enhancing energy efficiency. To facilitate the conversion of CO2 to COO- while concurrently suppressing HER in proton-rich acidic settings, it is imperative to grasp the underlying mechanisms of acidic electrolytes.This research demonstrated the correlation between hydronium ions and CO2RR by contrasting diverse CO2RR activities under varying electrolyte pH conditions, which dictate the reaction characteristics. The study presented an insight into the mechanisms of CO2RR and HER in acidic electrolytes. Additionally, the strength and interaction of intermediate compounds within the CO2 conversion pathway were verified using spectroscopy. A comparison was drawn regarding the CO partial current density between alkali cations of single-atom catalysts and metal catalysts. In an acidic environment, confirming FECO increases from 0 to over 90% for the same catalyst at pH 2.0, depending on electrolyte factors.

Furthermore, in an electrolyzer based on a gas diffusion electrode (GDE), exceptional CO selectivity of up to 96% was observed alongside stability lasting over 50 hours.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 09:56

Chair: Changsuk Yun (Changwon National University)

Synthesis of Heterometal Doped Silver Nanoclusters and Their Electrocatalytic Applications for Hydrogen Production

Hanseok Yi, Jiyeon Shin, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

A superatom is a cluster of atoms that mimics the properties of an element. Atom-precise metal nanoclusters (NCs) with protecting ligands are also considered one of the superatomic complexes. In NC systems, heterometal doping is a powerful method for tunning the physicochemical properties of homometallic NCs. While the heterometals doped into such NCs predominantly include transition metals with closed d-shells, the doping of open d-shell metals remains largely unexplored. Recently, we reported the first synthesis of a $[RhH@Ag_{24}(SR)_{18}]^{2-}$ (SR = thiolate) NC, in which a Rh atom with open d-shells ($[Kr]4d^8 5s^1$) is incorporated into the Ag_{24} framework by forming a RhH entity. Combined electrochemical and theoretical investigations showed that the RhH dopant was a superatomic construct of a Pd atom ($[Kr]4d^{10}$). To evaluate the dopant effects on hydrogen evolution reaction (HER), we synthesized $M@Ag_{24}(SR)_{18}$ (M = Ag, Pt, RhH) NCs with a similar atomic structure. Under acidic conditions, all doped Ag NCs showed comparable HER activities regardless of the dopants. However, the HER activities in alkaline conditions were found to be distinctly different depending on the dopants. Further kinetic isotope effect experiments and theoretical studies were performed to understand the origin of the dopant effects. Among the NCs, the $RhH@Ag_{24}(SR)_{18}$ NCs exhibited the highest HER activity, and its stability was confirmed through 24-hours constant potential electrolysis.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 10:03

Chair: Changsuk Yun (Changwon National University)

Electrochemical 5-hydroxymethylfurfural oxidation reaction (HMFOR) on defective NiOOH electro-catalyst

Juhyung Choi, Yun Jeong Hwang*

Department of Chemistry, Seoul National University, Korea

The growing consumption of poly(ethylene terephthalate) (PET) for producing plastic causes severe CO_2 emission, accelerating global warming. The production of poly(ethylene 2,5-furandicarboxylate) (PEF), capable of substituting PET, has been considered a sustainable measure. Electrochemical 5-hydroxymethylfurfural oxidation reaction (HMFOR) has attracted attention as a clean biorefinery process to produce the 2,5-furandicarboxylic acid (FDCA), which is considered a green precursor for PEF. Therefore, achieving efficient HMFOR promotes a circular economy with value-added products. Although Ni-based materials have been proven to be the most efficient catalyst, among other transition metal-based catalysts, their activities and reaction kinetics towards HMFOR need further improvement. Herein, we synthesized defective NiOOH (d-NiOOH) nanosheets with numerous oxygen vacancies by electrochemical-driven surface reconstruction of nickel molybdenum pre-catalyst. We found that d-NiOOH exhibits a high FDCA yield of 96.9 %, nearly 100 % conversion of HMF, and 98.1 % faradaic efficiency (FE) at 1.37 V (vs. RHE) for 1h 44m. In addition, Raman spectroelectrochemical studies supported the highly reversible phase regeneration kinetics of d-NiOOH during HMFOR, proving its high catalytic performance.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 10:10

Chair: Changsuk Yun (Changwon National University)

The Effects of mesoporous TiO2 layer for Photocatalytic Alcohol Oxidation Under Mild Conditions

Hyoeng Cheol Kang, Jongdeok Park[1], Jae-Joon Lee[1,*]

Energy & Materials engineering, Dongguk University, Korea

[1]Department of Energy and Materials Engineering, Dongguk University, Korea

Recent research efforts have focused on solar-assisted photoelectrochemical reactions to enable the oxidative decomposition of lignin and facilitate the production of value-added chemicals. However, the direct electrochemical oxidation of benzylic alcohol requires high applied potentials (>1.6 V) to achieve sufficient conversion, resulting in low selectivity, especially for aliphatic alcohols, and an inability to suppress side reactions. To address these challenges, a dye-sensitized photoelectrochemical cell (DSPEC) utilizing a N-oxyl radicals has been investigated. The aim is to improve both selectivity and conversion yield by employing non-stoichiometric amounts of the mediated catalyst under a reduced applied bias potential. In this study, our focus was on the fabrication of a high-performing photoelectrode using the photocatalyst tris(2,2'-bipyridyl-4,4'-dicarboxylic acid) ruthenium(II) (RuL3) immobilized on mTiO2 film. We aimed to determine the optimized thickness of the mTiO2 film to drive the oxidative cleavage of C(aryl)-Calkyl bond in 1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (LMC) in an organic media containing N-hydroxyphthalimide (NHPI) as a co-catalyst. The thickness of the mTiO2 was controlled using screen printing method on fluorine doped tin oxide (FTO) glass substrates, resulting in 1-mTiO2, 2-mTiO2, 4-mTiO2. We assessed the influence of mTiO2 thickness on NHPI catalysis including back electron transfer, recombination, and photocatalyst surface coverage. Furthermore, we investigated the product of yield of the reaction with varying thickness of mTiO2 to demonstrate the capability of charge transfer between photoanode to co-catalyst.

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 10:17

Chair: Changsuk Yun (Changwon National University)

[Withdrawal] Advancing PEM Water Electrolyzers: Surface Engineering of 1T′-Phase WS2 Nanosheets with Stabilized Ti3C2 MXene for Improved Hydrogen Evolution Reaction

Bee Lyong Yang

Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea

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

Oral Presentation for Young Electrochemists

Room 206+207 THU 10:24

Chair: Changsuk Yun (Changwon National University)

Interface Engineering for Enhanced Zinc Cobalt Sulfide Performance for Electrochemical Water Splitting

Mikiyas Mekete Meshesha, Bee Lyong Yang[*]

School of Advanced Materials Science and Engineering, Kumoh National Institute of Technology, GHS Co. Ltd., Korea

The innovative approach of integrating diverse components into a single heterostructure enhances the catalytic activity of both hydrogen evolution reactions and oxygen evolution reactions during the process of water splitting. In this research, a new hierarchically porous one-dimensional nanowire array, composed of zinc cobalt sulfide and molybdenum disulfide ($MoS_2@Zn_{0.76}$ $Co_{0.24}S$), was successfully created on a Ni foam substrate using a simple and efficient hydrothermal synthesis method. The inclusion of the metallic phase of molybdenum disulfide improves the electronic conductivity of $MoS_2@Zn_{0.76}$ $Co_{0.24}S$, leading to remarkably low overpotentials. Specifically, at current densities of 20, 50, and 100 mA cm^{-2}, the overpotentials for the oxygen evolution reaction are only 90 mV, 170 mV, and 240 mV, respectively. Similarly, for the hydrogen evolution reaction, the overpotentials at the same current densities in a 1.0 M potassium hydroxide solution are 169 mV, 237 mV, and 301 mV. The $MoS_2@Zn_{0.76}$ $Co_{0.24}S$ / Ni foam electrolyzer proves its exceptional capabilities as a catalyst in alkaline electrolyzers, operating efficiently at a mere 1.45 V and 10 mA cm^{-2}

Acknowledgments

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science, and Technology (MEST) [grant numbers: 2021R1A2C1006010], by the Technology development Program (Project No.: S2960707) funded by the Ministry of SMEs and Startups (MSS, Korea) and by the Technology development Program (RS-2023-00218808) funded by the Ministry of SMEs and Startups (MSS, Korea).

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

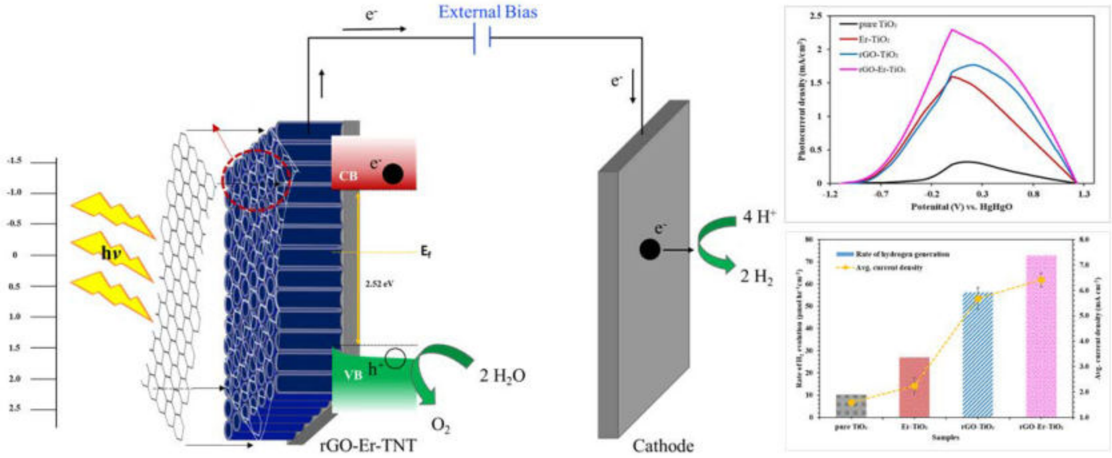
Oral Presentation : **ENVR.O-1**
General Session
Room 301 THU 09:20
Chair: Bupmo Kim (KENTECH)

Inorganic Photoelectrodes for Organic Pollutant Degradation and Hydrogen Production: Scale-Up Photocatalytic Reactor and Catalysts Design

Hyekyung Cho, Jeehye Byun[*]

Water Cycle Research Center, Korea Institute of Science and Technology, Korea

Due to the pressing issues of climate change and environmental pollution, the adoption of sustainable and efficient technologies has seen a remarkable increase. These technologies aim to mitigate environmental pollution and harness renewable energy sources. Photocatalysis has emerged as a promising solution to address this dual challenge, providing a unique platform for the degradation of organic pollutants and energy production. This presentation focuses on developments in scaling up inorganic photocatalysts and designing rotating reactors for organic pollutant degradation under solar irradiation. Furthermore, it explores the synthesis of binary and ternary nanocomposites were synthesized based on TiO2 nanotubes as photoelectrodes, incorporating lanthanide metals and carbon materials to investigate their potential in hydrogen production through photoelectrochemical processes.


External Bias
e⁻
e⁻
-1.5
-1.0
-0.5
0
0.5
1.0
1.5
2.0
2.5
hv
CB
e⁻
E_f
2.52 eV
VB
h⁺
2 H₂O
O₂
rGO-Er-TNT
e⁻
4 H⁺
2 H₂
Cathode
pure TiO₂
Er-TiO₂
rGO-TiO₂
rGO-Er-TiO₂
Photocurrent density (mA/cm²)
Potenital (V) vs. HgHgO
-1.2
-0.7
-0.2
0.3
0.8
1.3
0
0.5
1
1.5
2
2.5
Rate of hydrogen generation
Avg. current density
Rate of H₂ evolution (μmol hr⁻¹cm⁻²)
Avg. current density (mA cm⁻²)
0
10
20
30
40
50
60
70
80
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
pure TiO₂
Er-TiO₂
rGO-TiO₂
rGO-Er-TiO₂
Samples

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

General Session

Room 301 THU 09:40

Chair: Bupmo Kim (KENTECH)

A pervaporation process for separation of mixtures and purification and recycling of chemicals using graphene oxide membranes

Byeongho Lee, Choonsoo Kim[1,*]

Environmental engineering, Kongju National University, Korea

[1]*Department of Environmental Engineering, Kongju National University, Korea*

Membrane technology for chemical dehydration, purification, and the separation of liquid and vapor mixtures, known as pervaporation or pervaporative separation, has been gaining significant attention as a promising alternative to traditional distillation methods for the separation process. Pervaporation, when applied to liquid-phase feeds, and vapor permeation, for vapor-phase feeds, are membrane-based processes designed to selectively separate mixtures using a non-porous or porous membrane as a selective barrier between the feed and permeate. This research specifically explores the use of a graphene oxide (GO) membrane for separating a binary vapor mixture of water and alcohol through the vapor permeation process. The GO membrane demonstrates a remarkable ability to selectively permit the permeation of water due to its inherent hydrophilic properties. Consequently, it is evident that the GO membrane holds great promise as a cutting-edge membrane technology for the purification of alcohol compounds, heralding it as a potential candidate for the next-generation pervaporation membrane.

Oral Presentation : **ENVR.O-3**
General Session
Room 301 THU 10:00
Chair: Bupmo Kim (KENTECH)

Sulfate-rich wastewater induces the sulfur aging of microplastics in the anaerobic digestion system

Jihee Kim, EunJu Kim[*]

Korea Institute of Science and Technology, Korea

Anaerobic digestion (AD) process, one of the sewage sludge treatment processes, has been widely applied in organic waste treatment due to its ability to biologically stabilize sludge, eliminate pathogens, and produce biogas. During the AD process, sulfide production is inevitable due to the sulfate reduction or the decomposition of sulfur-containing compounds (e.g., protein) in the sludge. In fact, sulfide can act as a common nucleophile and reductant in diverse environments, especially anaerobic systems, suggesting the potential transformation of microplastics (MPs) by sulfide treatment. The study of sulfur aging (or weathering) of MPs in anaerobic environments is still insufficient compared to MP aging in aerobic environments, however, the sulfur aging on MPs in a sulfide-rich environment has been recently investigated. This study aimed to investigate the sulfur aging of MPs during the AD processes in sulfate-rich wastewater, associated with biological sulfate reduction by sulfate-reducing bacteria, and further its impact on metal adsorption. In order to verify the sulfur aging of MPs during the AD process, the batch experiment was conducted to simulate the AD conditions. We observed the sulfur aging of MPs during the AD process using electron microscopy, X-ray photoelectron spectroscopy, and Fourier transform infrared spectroscopy, along with the changes in microbial communities by analyzing the 16S rDNA and dsrB genes. We further tested the impact of sulfur aging on metal-MP absorption. This study suggested the possibility of sulfur aging of MPs during the AD process with the input of sulfate-rich wastewater such as the industrial wastewater treatment plants, which can improve the understanding of the transformation of MPs under anaerobic environments.

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

General Session

Room 301 THU 10:20

Chair: Bupmo Kim (KENTECH)

Photoelectrochemical activation of BiOBr in bromide solution for stable and improved photoelectrochemical conversion efficiency

Wonjung Choi, Yiseul Park*

Pukyong National University, Korea

Photoelectrolysis is a sustainable technique with immense potential for the degradation of aquatic contaminants and the generation of valuable energy resources. BiOBr is being estimated as a promising photoelectrocatalyst owing to its narrowed bandgaps and structural durability, and numerous research efforts are underway to enhance its photoelectrochemical performance. In this research, we provide experiment evidence that the use of bromide solution for electrolyte significantly enhances the electrochemical performance and contaminant breakdown capabilities of BiOBr, without any physical/chemical modification. At the initial of photoelectrolysis, the observed current density records at 40 μA·cm^{-2} but over the course of 5 hours, the current density experiences an improvement of around 38 times, reaching 1.5 mA·cm^{-2}. Subsequently, after 20 hours, the current density further increases to around 3 mA·cm^{-2}. Furthermore, while comparing with the results in the perchlorate solution, it is seen that the oxidation rate of arsenite (As(III)) is more than 4 times higher in the bromide solution. While the specific mechanism of the performance enhancement has yet to be identified, the findings of this work highlight the possibility of enhancing the photoelectrochemical performance of BiOBr. It has significant implications for the development of cost-effective and environmentally sustainable methods for photoelectrolysis systems and solar fuel production.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Oral Presentation : **ENVR.O-5**
General Session
Room 301 THU 10:40
Chair: Bupmo Kim (KENTECH)

Water pollutant redox reactions using photo-charged inorganic catalysts membrane filters in the absence of irradiation

Jiyeon Park, Hyunwoong Park[1,*]

Energy Engineering, Kyungpook National University, Korea
[1]School of Energy Engineering, Kyungpook National University, Korea

Solar energy has several advantages, and photocatalytic research in the presence of light has attracted significant interest. However, depending on the situation, sunlight is limited (e.g., climate or night). These limitations can be solved in part by using photocatalysts with special characteristics in the dark. Photo-charged TiO2/WO3 catalysts, which are likely water treatment, have been demonstrated via oxidation reactions in the dark. In this work, photo-charged TiO2/WO3(TW) membrane filters for water pollutant remediation are evaluated in the dark. The interaction between water contaminants and TW catalysts is demonstrated in this study. This membrane filter is simple to make and environmentally friendly because can be easily reusable and recharged without the requirement of additional physical and chemical separation steps.

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Ring-opening Copolymerization Using a Chromium(III) catalyst with a Readily Available Aminotriphenolate Ligand

Seungyeon Jeong, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

An alternating ring-opening copolymerization of cyclic anhydrides with a series of epoxides using a new chromium(III) complex (2) with a readily available aminotriphenolate ligand ($L^{tBu,tBu}$) was studied. The single crystal structure of 2 has octahedral geometry in contrast to the general trigonal bipyramidal geometry of transition metal aminophenolate complexes. The complex 2 and a cocatalyst (bis(triphenylphosphine)iminium chloride or 4-dimethylaminopyridine) as a binary catalytic system produced perfectly alternating polyesters with high molecular weights and low dispersity at high selectivity. Also, differently substituted monomers could be applied and the thermal properties (T_g up to 180 ℃) of the resulting polyesters tuned by the monomer selection.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Chiral Polymer Coatings on Substrates *via* Surface-Initiated RAFT Polymerization Under Ambient Conditions

Yerim Lee, Kyung-sun Son[1,*]

Chungnam National University, Korea

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

In this study, chiral polymers based on amino acids were successfully grafted on the substrates by surface-initiated reversible addition-fragment chain transfer polymerization using oxygen (O_2-SI-RAFT) under ambient conditions. Chiral monomers were synthesized using methacrylic anhydride and L/D-amino acids, and chiral polymers were grown on titanium and glass substrates. Block copolymer brushes were also polymerized through chain extension. This is the first report of RAFT polymerization of chiral monomers on the substrate, and the first confirmation of chirality through on-surface CD spectroscopy.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Bridge-rich and loop-less hydrogel networks through suppressed micellization of multiblock polyelectrolytes

Jihoon Han, Younsoo Kim[1,*]

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

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

Most ABA triblock copolymer-based physical hydrogels form three-dimensional networks through micellar packing, resulting in decreased elasticity. This effect can be mitigated by maximizing the fraction of elastically effective bridges in the hydrogel network. Previous observations have shown that the ratio of bridges increases with increasing the relative length of the middle block and the polymer concentration. However, despite the numerous efforts, there was a limit to maximizing the fraction of bridges based on the loop-rich micelle structure. Herein, we report polyelectrolytes complex hydrogels with network constructed by designing block copolymers with a structure that maximizes the entropy penalty of micellization. These copolymers directly self-assemble into branched and bridge-rich network units (netmers) instead of forming self-entangled independent micelles. As a result, netmers are hierarchically stacked to create a bridge-rich network, increasing hydrogel elasticity.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

A research on Polymer Electrolyte of Episulfide Monomer Using Thermosetting

Minhyuk Jeon*, Wansu Bae[1], Sungjun Park[1], Hohyoun Jang[2]

Applied chemistry, Konkuk University, Korea

[1]*Applied Chemistry, Konkuk University, Korea*

[2]*Konkuk University, Korea*

As most industries are driven by batteries, the importance of secondary batteries is increasing day by day. Among them, as research on electrolytes progresses, polymer electrolytes based on ethylene oxide (PEO) oligomers and lithium salts as polymer electrolytes have attracted great interest to develop the most modern lithium secondary batteries. However, due to the strong interaction of lithium and oxygen in the pure polymer electrolyte, there is a problem of a low lithium transition number, and in the case of an epoxy resin, it takes a lot of time to cure at low temperature. Here, using LiFSI as an initiator and using an episulfide structure in which oxygen in epoxy is replaced with sulfur, it is easy to apply fast curing at a low temperature and can show improved conductivity than PEO due to lower competitive strength with lithium ions. shows. The physical and chemical properties of the cured material were investigated through FT-IR, H-NMR, and TGA, and the efficiency was also measured through electrochemical analysis using EIS, CV, and LSV using a gel polymer electrolyte containing a solvent.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Rational Design of Polymer material with dual functionality for Solution-Processed TADF-OLED

MinJi Kang, Dong Hoon Choi[*]

Department of Chemistry, Korea University, Korea

In this study, we propose poly(phenylethyl-9H-3,9'-bicarbazole) (PPBCz) that can be used for solution processed thermally activated delayed fluorescence (TADF) OLED. Solution-processed OLEDs have several advantages, such as, ease of large-scale fabrication, low-cost manufacturing, and reduced material consumption. In the case of polymer, it exhibits high thermal stability and possess excellent film-forming capabilities due to their high solubility, making them well-suited for solution-processed OLED materials. The PPBCz has HOMO and LUMO level of -2.06 eV and -5.41 eV, respectively. And PPBCz has high triplet energy (2.78 eV), it is a multifunctional material that suitable for host or hole transport material (HTM). The device was fabricated using 6 wt% t4CzIPN, a green TADF emitter. Both the device using PPBCz as a host and the as a HTM showed decent device performance. In addition, it showed an improved efficiency roll-off when used as HTM. These results show that PPBCz can implement dual functionality that can be used in both host and HTM.

Poster Presentation : **POLY.P-6**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

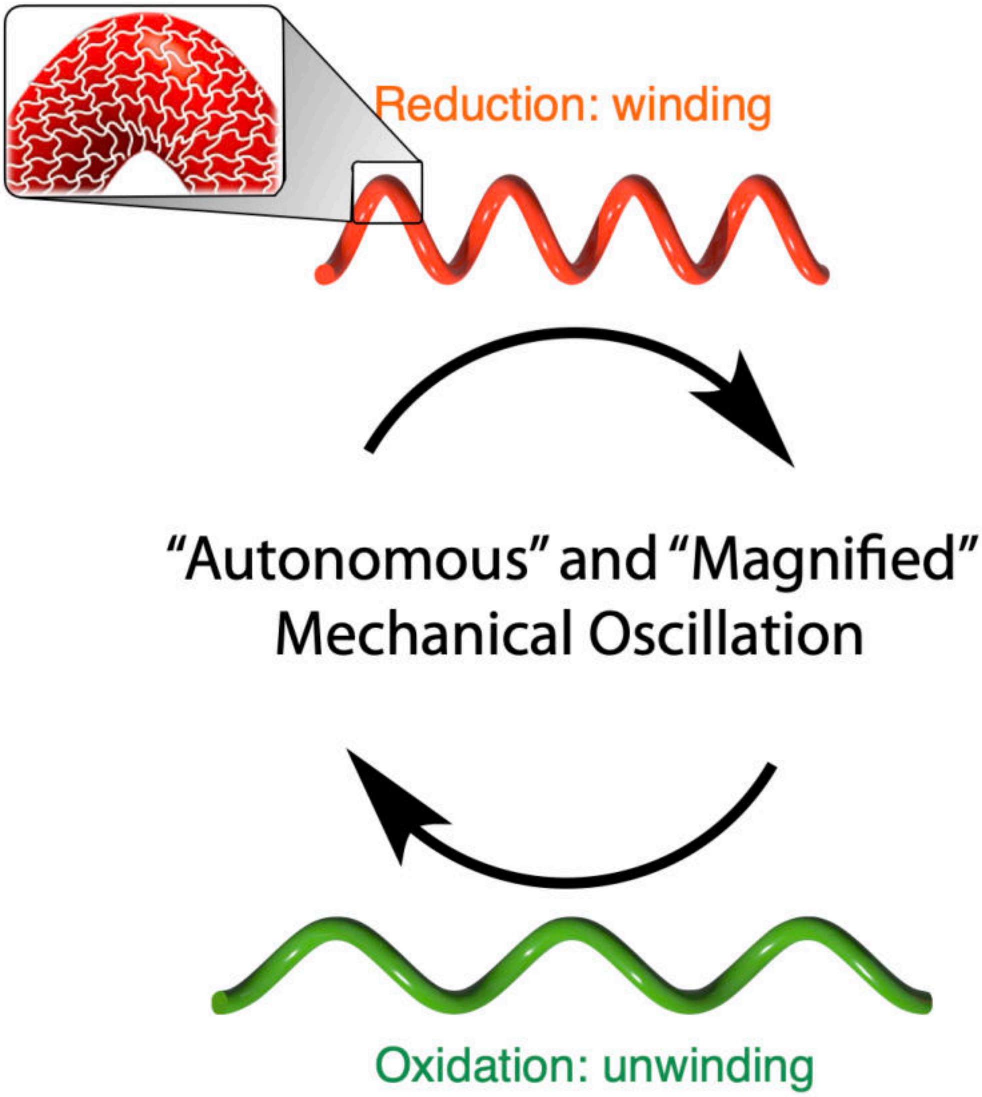
Helical-shaped Self-oscillating Gels showing Autonomous and Magnified Mechanical Oscillation

Taehun Chung, Ryo Yoshida[1], Younsoo Kim[*]

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

[1]*Department of Materials Engineering, The University of Tokyo, Japan, Japan*

Self-oscillating gels have become a distinguished class of smart soft materials because they undergo spontaneous and cyclic swelling-deswelling changes without on-off switching of external stimuli. However, their practical applications of them are still limited due to a small change and non-directional actuation by isotropic deformation. Herein, to improve the degree of deformation, we report an unprecedented method to convert an isotropic deformation into anisotropic and unidirectional deformation of gel. As a result of introducing a three-dimensional periodic gradient structure by photopolymerization into the gel network, a helical-shaped gel could be synthesized. The helical-shaped gels exhibited amplified uniaxial winding and unwinding during the Belousov–Zhabotinsky (BZ) reaction. In addition, they showed a significant change in length compared to the conventional rod-shaped gel. This presentation will discuss synthetic strategy, structure analysis, and improved self-oscillation of helical-shaped gels.


Reduction: winding
"Autonomous" and "Magnified"
Mechanical Oscillation
Oxidation: unwinding

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Investigating Thermodynamic Trends in Gold Nanoparticles: Effects of Size and Molecular Weight of Ligand

Dong Jin Kang, **Hongseok Yun**[1,*]

College of Natural Sciences / Department of Chemistry, Hanyang University, Korea

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

Attaining well-organized arrays of nanoparticles (NPs) with controlled packing symmetry and interparticle spacing holds great significance in the creation of intricate metamaterials. In this study, we present the self-assembly behavior of gold nanoparticles functionalized with thiol-terminated polystyrene chains (Au@PS NPs), wherein the assembly behavior is determined by NP size and the molecular weight of PS ligand. Our study focuses on understanding the relationship between the packing symmetry of Au@PS NP and their thermodynamic properties, characterized by transmission electron microscopy and differential scanning calorimetry, respectively. Through this approach, we attempt to clarify the differences in thermodynamic behavior between polymeric ligands confined within the packing symmetry of NP cores and unbound free polymers.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Enzyme-Catalyzed Self-Assembly for ER Targeting

Jihun Roh, Beom jin Kim[1,*]

University of Ulsan, Korea

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

Enzyme-catalyzed self-assembly (ECSA) is an advanced methodology that spatiotemporally regulates supramolecular self-assembly through an enzymatic reaction.[1] Because the enzyme expression level varies across the cell types, it is possible to induce the peptide self-assembly within only cancer cells, when we use the enzyme overexpressed in cancer cells. Here we report that the novel strategy for targeting endoplasmic reticulum (ER) of cancer cell. Alkaline phosphatase (ALP) is overexpressed in various cancer cells, allowing ECSA within cancer cells. We designed the peptide building block for self-assembly to target the cancer cells without any damage of normal cells. In addition, we conjugated the p-toluenesulfonyl (Ts) group to the peptide building block for ER targeting, because Ts group leads to target the ATP-dependent potassium channel that in the ER.[2] As a result, we success to achieve the selective inhibition of cancer cell with ER targeting.Reference: 1. Kim, B. J.* Chem. Asian J. 2022, 17, e202200094.2. Yi Liu.; Hao-Ran Jia.; Xiaofeng Han.**; Fu-Gen Wu.* Smart Mater. Med. 2021, 2, 334-349.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Mechanical properties and impact strength of PLA/PSMA ionomer blends

Dahye Kim, Joon-Seop Kim*

Department of Polymer Science and Engineering, Chosun University, Korea

Biodegradable PLA is difficult to use as a general-purpose polymer due to its low glass transition temperature and brittleness. Therefore, in this study, poly(styrene-co-methacrylate) ionomer with a high glass transition temperature was blended with PLA to overcome the disadvantages of PLA. The ionomer was neutralized with Na+ or Li+, and the content of ionic groups was 10 mol% or 21 mol%. The physical properties of these blends were measured using DMA and Izod impact testers. The storage modulus increased rapidly when the ionomer content of the blend was less than 15 wt% at 100 to 150 °C, but increased slowly when the ionomer content was 15 wt% or more. However, the impact strength decreased rapidly when the ionomer content of the blend was less than 10 wt%, and there was little change even when the ionomer content was increased. From these results, we concluded that the thermal properties were improved because the PLA interacted with the ionomer, but the impact strength of the PLA was lowered because the ionomer existed in the PLA matrix in a phase-separated form.

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Structure and phase behavior of ABA-type triblock copolymer induced by random sequence ensemble

Jimin Yoo, Myungeun Seo[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Amphiphilic copolymers composed of hydrophobic and hydrophilic monomers have been reported to form a bilayer-folded lamellar (Lf) mesophase in water, driven by local curvature arising from sequence mismatching problems in random sequences. This process can be seen as the emergence of order from disorder in random sequence ensembles. In this study, we aim to immobilize this folding structure by introducing rigid domains at the chain ends of amphiphilic random copolymers to observe the resulting phase behavior. We used reversible addition–fragmentation chain transfer (RAFT) polymerization to synthesize ABA-type triblock copolymers with a polystyrene block attached to the ends of the amphiphilic random middle block. These copolymers were prepared in high-concentration solutions and their structures were analyzed using small-angle X-ray scattering (SAXS). Depending on the styrene fraction within the chains, we observed the presence of either folding structures or the architecture of triblock copolymers. These triblock hydrogels are expected that it can be used as an soft material that exhibits improved physical properties.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of a Trisaryl Phosphoric Triamide-Based Resin In Quartz Crystal Microbalance Sensor for Detection of Sulfur Mustard Simulant

Jin Hyun Park, Han yong Bae, Changsik Song*, Jaeyoung Heo[1]

Department of Chemistry, Sungkyunkwan University, Korea

[1]*chemistry, Sungkyunkwan University, Korea*

Chemical warfare agents pose a persistent threat to human safety, with bis(2-chloroethyl)sulfide (SM) being one of the most dangerous substances capable of causing serious harm. Detecting SM gas is vital, but current methods face challenges like high-temperature requirements and limited selectivity, mainly because of the lack of receptor development. To address this issue, we present a trisaryl phosphoric triamide-based resin receptor, preferentially interacting with a sulfur mustard simulant (2-CEES) through dipole-induced dipole interactions. The receptor was synthesized simply using an amine and triethyl phosphate, and its coating properties were enhanced with an epoxy chemistry. Evaluated using a quartz crystal microbalance (QCM), the receptor's superior structure was confirmed by observing reactivity variations with the number of phosphoramides. The receptor shows better reactivity to 2-CEES vapor than previously known poly(epichlorohydrin), and showed selectivity to other volatile organic compounds (VOCs). Moreover, its durability was evident even after 30 days post-coating. The receptor's potential applicability would extend to array sensors, sound acoustic wave (SAW), chemo-resistive, and chemocapacitive sensors, promising in advancements for chemical warfare agents detection.

Poster Presentation : **POLY.P-12**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)] by the Stille Coupling Reaction of 2,5-Dibromosiloles with Bis(tributylstannyl)acetylene reagent and Electrochemical Characterization

Ji hun Lee, Young Tae Park[1,*]

Keimyung University, Korea

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

Dialkyl(R = Et, or iso-Pr, or *n*-Hex)-bis(phenylethynyl)-silanes were reacted with lithium naphthalenide, anhydrous zinc chloride, and *N*-bromosuccinimide (NBS) to obtain 1,1-dialkyl(R = Et, or iso-Pr, or *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles, respectively. Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)], conjugated polymers containing with silolene and acetylene, were synthesized through the Stille coupling reaction of 1,1-dialkyl-2,5-dibromo-3,4-diphenyl-siloles and bis(tributylstannyl)acetylene as co-monomers, in the presence of toluene as solvent and dichlorobis(triphenylphosphine)palladium as catalyst. The crude products were purified by precipitation with methanol and then furthermore purified by extraction with chloroform. The obtained polymeric materials were analyzed by ^{1}H, ^{13}C, ^{29}Si NMR, FT-IR, GPC and UV-vis spectroscopy. The electrochemical properties of the prepared polymers as anode materials for lithium-ion batteries was also studied.Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-13**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Carbazole based crosslinkable hole transport materials for solution processed quantum dot light emitting diodes.

Hyeonjoo Lee, Do-Hoon Hwang[1,*]

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

There are a vacuum deposition method and a solution process method for manufacturing a multi-layered quantum dot light emitting diode (QLED).The solution process has the advantages of being relatively inexpensive, less time consuming and highly material efficient.In the case of QLED, since the HOMO energy level of the light emitting layer (EML) is low, a low HOMO energy level of the HTL (Hole Transfer Layer) is required for high hole mobility and excellent device efficiency.However, in the case of solution process HTL, there is a problem that the lower and upper layers can be mixed.Poly-9-vinylcarbazole (PVK) has a low HOMO energy level of -5.9eV and is used as a QLED HTL, but has low hole mobility.In addition, the existing PVK is used as an orthogonal, but there is a limitation that it can be used only when the EML solvent is toluene and cannot be used in the case of other solvents such as chlorobenzene.In order to expand the solvent, a thermal crosslinker was introduced to design and synthesize new materials.As a result, HTL materials with appropriate HOMO energy levels, high hole mobility, and high solvent resistance to various solvents that can replace PVK for QLEDs were synthesized.

Poster Presentation : **POLY.P-14**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Facile Diels–Alder Reaction–Aromatization Reaction Using Biomass-derived Furanic Dienes for Supramolecular Phthalimide Networks

Hong Okbi, **Changsik Song**[1,*]

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

The core of phthalimide is an important material that can be applied to organic, pharmaceutical, and material fields. Conventional phthalimides were synthesized by the DA adduct through the Diels-Alder reaction of furan and maleimide and proceed with dehydration under thermal and acid conditions. However, these areas need to be improved due to the harsh reaction conditions and long reaction times. In this study, we devised a facile and convenient synthetic pathway (no heat or acid/catalyst needed) to produce phthalimides. The N-carbamate group was introduced directly at the C-2 position of furan via thermal Curtius rearrangement. The N-carbamate group increased the HOMO energy level and showed an improved DA reaction rate compared to the conventional furfuryl furan. And under mild DA reaction conditions, our material proceeded to aromatize, confirming the synthesis of phthalimide groups. In summary, we have presented a novel biomass-based phthalimide synthesis method, which is expected to be applied to various fields including phthalimide motifs.

Poster Presentation : **POLY.P-15**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Sustainable eco-friendly polyurethane using carbon dioxide capture and furan-based biomass polyol at the same time

Ji won Jang, Hong Okbi[1], Changsik Song[2,*], Eun Joo Kang[3,*], Junhyeon Choi[3]

Department of chemistry, Sungkyunkwan University, Korea
[1]*Chemistry, Sungkyunkwan University, Korea*
[2]*Department of Chemistry, Sungkyunkwan University, Korea*
[3]*Department of Applied Chemistry, Kyung Hee University, Korea*

Polyurethane is an essential polymeric material used in various modern industrial fields because it has high chemical stability and can freely adjust its physical properties according to the combination of an alcohol group and an isocyanate. However, since most of the raw materials used to make polyurethane use resources derived from limited petroleum resources, price volatility is high, and it causes various environmental pollutants such as carbon dioxide, a significant greenhouse gas. To overcome these problems, research on polymer materials using biomass-derived materials and carbon dioxide capture technology that separates and captures carbon dioxide from the atmosphere has been actively conducted. This study synthesized several eco-friendly polyurethanes using biomass-based polyols (FBP) and carbon dioxide-trapping polyols (Diol, Triol). The synthesized eco-friendly polyurethane has a high green carbon content of over 90%, which is very high compared to existing eco-friendly polyurethanes by simultaneously introducing carbon dioxide capture technology and biomass material. This study used the synthesized polyurethane as an adhesive for various materials. However, it is expected to be applied in various fields other than adhesives.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **POLY.P-16**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

PHOTOLYSIS OF EUMELANIN WITH THE HYDROGEN PEROXIDE

Ghanyatma Adi Baskoro, Beom jin Kim[1,*]

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

Eumelanin, an abundant black pigment found in many parts of living organisms, has drawn a lot of attention in the field of photoactive biomaterials. The key reasons are its widespread UV-visible absorption, relatively small band gap, and simplicity of synthesis. In this work, we proposed a concept that utilizes the photogenerated species formed when the eumelanin was illuminated with blue light to generate reactive oxygen species (ROS) by the presence of H_2O_2. The generated ROS were then prone to promote the degradation of eumelanin. Here, we provide evidence that the eumelanin was possible to be completely degraded in a brief amount of time when exposed to a relatively low concentration of H_2O_2 (less than 1 w/w%) under blue light illumination. Furthermore, we were able to degrade the innate eumelanin in black human hair by employing this strategy. These findings may hold promise for further understanding eumelanin photophysical properties and broadening the horizon for eumelanin applications as photoactive biomaterials.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Fabrication of patterned nanofibers through controlled liquid crystal templating via electric field

Jeong Yeon Han, Changjae Lee, Dong Ki Yoon*

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

Liquid crystals (LCs) can be a template for aligning functional guest materials because their tunable orientation originates from their unique property to respond to external stimuli. We fabricate the patterned fiber array from the electrically modulated (in-plain) nematic LC template using the chemical vapor polymerization (CVP) method. Under an electric field, an induced defect structure with a winding number of -1/2 contains a periodic zigzag disclination line. It is known that LC defect structures can trap the guest materials such as particles and chemicals. However, the resulting fibers grow along the LC directors, not trapped in the defects. To show the versatility of our platform, nanofibers are fabricated on patterned electrodes representing the alphabet letters "CVP" and different electrode distances. In addition, by comparing the contact angle from the fibril array with the hydroxyl group or semi-fluorinated group, it is confirmed that the structural property can amplify the chemical property. The resultant orientation-controlled fibers will be used in controllable smart surfaces that can be used in sensors, electronics, photonics, and biomimetic surfaces.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Hight Molecular Weight Poly(L-Lactic Acid) by using Tin and Nickel Catalyst

Shin Hye Park, Longhai Piao*, Yunseo Park, Yejin Jeong, Sungho Yoon[1]

Department of Chemistry, Kongju National University, Korea

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

shin hye Park, Longhai Piao*, yun seo Park, ye jin Jeong, sangho YoonDepartment of Chemistry, Colleague of Natural Science, Kongju National University.Poly (L-Lactic acid) (PLLA) has been used in a variety of consumer products such as food packaging, drinking straws and 3D printing filament, because it is considered as an environmentally friendly alternative to traditional plastics. Hight molecular weight PLLA is synthesized via ring-opening polymerization of L-lactide monomer, which is produced by the thermal depolymerization of oligomeric PLLA. The synthesis of L-lactide involves challenges, such as high raw material loss and significant synthesis time, during the conversion of lactic acid to L-lactide monomers. Additionally, issues arise due to the occurrence of racemization reaction to produce meso form lactide, which reduce the yield of L-Lactide. This study aims to increase the yield of L-Lactide while achieving high molecular weight PLLA. Tin and Nickel compounds were employed as catalysts for both depolymerization of PLLA oligomers and polymerization of L-lactide. And the reaction conditions were modified to discover the optimal synthesis conditions for increasing L-Lactide yield. For the polymerization reaction, the influences of the catalyst concentration and reaction time to the molecular weight were investigated in order to obtain high molecular weight PLLA. These authors equally contributed to this manuscript.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

A novel siloxane-based transdermal delivery polymer formulation

Miyeon Jeong, Dokyoung Kim[1,*]

Precision medicine, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Transdermal drug delivery system (TDDS) is a route of drug administration allows patients to readily intake therapeutic agents through the skin. It could avoid the first-pass metabolism, which occurs upon oral administration, and absorb without pain due to its non-invasive properties. So, many formulations have been developed to enhance the solubility and permeability of the various drugs that could not be easily transferred to the skin. Polymer, one of the formulations for TDDS, could control the release and reduce the side effects due to its high stability and biocompatibility. However, the previous polymers, such as polydimetheysiloxane (PDMS), polylactide-co-glycolide (PLGA), and hyaluronic acid, are either too hydrophilic or hydrophobic. Hence, we reported the most outstanding polymer (C2 polymer) discovered from our polymer series (PDDS) to administer the drug through the skin. PDDS was polymerized by the acidic initiator (acetic acid (AA), citric acid (CA), trifluoroacetic acid (TFA), or hydrochloric acid (HA)) opening the cyclic ring structure of the monomer (2,2,5,5-tetramethyl-2,5-disila-1-oxacyclopentane (TDOP)) to a linear structure. In this one-pot synthesis method, polymers of these series were prepared by changing polymerization temperature and molar equivalent as well as the type of initiator. We showed that the SN-38 loaded C2 polymer ([TDOP]:[CA]=13.8:1, 80°C) could enhance skin penetration and in vivo anti-cancer effects more than the free drug. In conclusion, we expected that the C2 polymer will be utilized as the most promising polymer of PDDS with no toxicity for TDDS.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Characterization of BDT based Polymer for Organic Thermoelectrics

Youjin Kim, **Do-Hoon Hwang**[1,*]

Pusan National University, Korea

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

Organic thermoelectric materials have the ability to convert heat into electricity, making them increasingly important in energy conversion and management. These materials are used in a variety of applications due to their flexibility and light weight, and are receiving great attention in fields such as solar cells, heat energy recovery devices, and wearable electronic devices. In this study, the main characteristics and factors affecting the performance of organic thermoelectric materials were analyzed. In this study, we observed changes in the performance of thermoelectric devices according to changes in the heterocycle of BDT-based polymers. As the heterocyclic atom size increases, the energy band gap decreases and the PF value becomes better.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Highly Efficient Green Homoleptic Ir(III) Complexes Approaching 21% of EQE by Solution-processed for Green PHOLEDs with Higher Efficiency

Al-amin Md, Yeong Soon Gal[1], Sung-Ho Jin[2,*]

Department of Chemical Education, Pusan National University, Bangladesh
[1]*Department of Fire Safety, Kyungil University, Korea*
[2]*Department of Chemical Education, Pusan National University, Korea*

Over the last few years, phosphorescent organic light emitting diodes (PHOLEDs) have been improved on the application of next-generation flat-panel displays, because of strong spin-orbit coupling, complexes with transition heavy metals as like Ir(III) complexes. In this study, two homoleptic iridium(III) complexes were designed and synthesized. Their thermal, photophysical, electrochemical, and electroluminescence characteristics were fully characterized. Both complexes exhibited featureless emission spectra with the maximum photoluminescence at 529 and 513 nm with high photoluminescence quantum yields of 88% and 85%. Notably, electron transport layer optimized devices using mer-MECF as a dopant exhibited maximum external quantum efficiency of 18.6% and 21.1% and a maximum current efficiency of 62.4 and 71.4 cd A-1. The introduction of different functional groups an effective approach to molecular designing Ir(III) complexes for high quality green solution-process PHOLEDs.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Reprocessable Polyvanillin-Based Resin via Imine Formation and Reductive Amination

Soyeon Kim, Byungjin Koo*

Department of Polymer Science and Engineering, Dankook University, Korea

Lignin is a polymer responsible for the woody and fibrous part of plants, obtained from byproducts of wood processing. Comprising various aromatic ring compounds, intricate structure of lignin can serve as a crucial building block for creating high-valued materials through processes like depolymerization or refinement. Among the phenolic derivatives from lignin, "vanillin," one of the phenolic derivatives from lignin, is widely used as a flavoring agent but high glass transition temperature (T_g) of vanillin-based polymer has led to research on its potential as an eco-friendly substitute for styrene. Herein, we reported the synthesis of homopolymers based on vanillin methacrylate (VMA) via RAFT polymerization and the resin based on imine bonding. The aldehyde moiety in VMA-based polymers induced cross-linking bonds when reacted with primary amine. This imination process offers the advantage of reacting in just a few seconds even at room temperature, enabling highly efficient resin production. The hydrolysis property of imine bonds under acidic conditions demonstrated that the resin can reversibly revert to homopolymers, implying its reprocessability. Lastly, due to the susceptibility of imine bonding to moisture in various industrial applications, we transformed imine linkages into amine bonding via reductive amination, making it permanently tolerant to moisture in different environments. We speculate that our fully bio-based resin using vanillin and cadaverine can be adapted for a wide range of applications, as it can be reprocessed or permanently altered as needed.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Transfer and Amplification of Helical Chirality in Hierarchical Self-Assembly System

Jun Su Kang, Kangseok Kim, Myungeun Seo*

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

Helical structures are prevalent in nature and play an essential role in living organisms. The functionalities of these, such as duplication and recognition, are derived from the hierarchical self-assembly of chiral building blocks across multiple length scales. Numerous studies have explored the transfer and amplification of chirality from molecules to helical assemblies and polymeric chains within self-assembly systems. However, there has been limited exploration of how helical chirality can be transferred and amplified to higher levels of architectures beyond molecular chiral sources. Here, we explore the transfer and amplification phenomena of helical chirality during the hierarchical self-assembly process, which leads to the formation of superhelices from helices. Employing chiral and achiral triarylamine (TAA) derivatives, we monitor the development of TAA co-assemblies resulting from dynamic chiral communication between the helices. We will discuss how temperature-dependent molecular and helical dynamics influence supramolecular chirality in the context of the emergence of multiscale chirality.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Cationic CO_2-based Polycarbonate synthesized by Graft Copolymerization

Gyu ri Kim, Nam-kyun Kim*

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

Recently, there has been a growing concern over environmental issues stemming from carbon dioxide emissions and plastic contamination. To address this pressing matter, we tried to develop synthetic method for preparation of aliphatic polycarbonates utilizing carbon dioxide as a fundamental component of the polymer structure. In this study, we synthesized a backbone with tertiary amine initiation points, enabling graft CO_2 polymerization, using the RAFT (Reversible Addition-Fragmentation Chain-Transfer) polymerization method. Subsequently, graft polymerization on the backbone using CO_2 and propylene oxide were conducted. The structure and molecular weight of the polymer were evaluated by 1H-NMR and SEC (Size Exclusion Chromatography) as a result.

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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

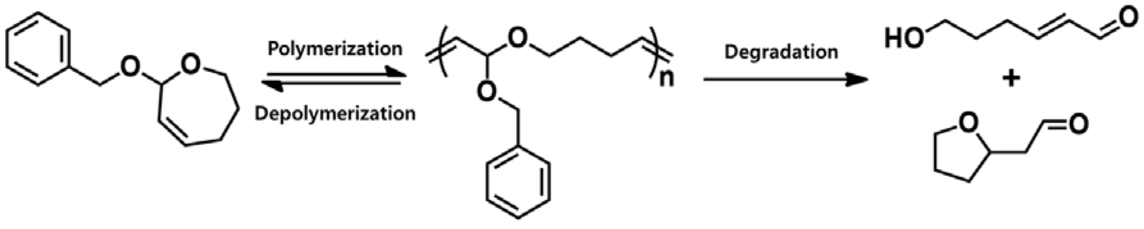
Depolymerizable and degradable polymer from cyclic acetal via entropy-driven ring-opening metathesis polymerization

Dayong Song, Cheoljae Kim[1,*]

Chemistry, Chungbuk National University, Korea

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

We demonstrated the polymerization and depolymerization of low strained 7-membered cyclic olefin via ED-ROMP. Direction of the polymerization and depolymerization was controlled by the reaction temperature and concentration in the equilibrium system: polymerization in high concentration at low temperature and depolymerization in low concentration at high temperature. Additionally, our monomer contained acid-labile acetal functionality, and this provides the degradable functionality overall polymer backbone.



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

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of Proton Conductive and Anti-Poisoning Ionomers for High Temperature Polymer Electrolyte Membrane Fuel Cells

Jungwoo Han

Department of chemistry, Sungkyunkwan University, Korea

Fuel cells are promising devices for environmentally friendly clean energy. Currently, low temperature polymer electrolyte membrane fuel cell (LT-PEMFC) with Nafion® as a membrane appears to be the most widely utilized. However, LT-PEMFC has disadvantages such that the operating temperature is limited to 100 °C under humidification conditions, and a water management system is also required, which can be overcome if operated at high temperatures. Phosphoric acid-doped polybenzimidazole (PA-doped PBI) is a promising material for a high temperature polymer electrolyte membrane fuel cell (HT-PEMFC). However, PA leakage due to the weak interaction of PBI-PA causes performance deterioration. Here, we developed a novel ion-pair coordinated polymer of intrinsic microporosity (PIM) polymers that showed higher PA doping and PA retention than PBI. As well as the strong interaction with PA, ion-pair-PIMs have good thermal stability at above 200 °C. We believe that ion-pair-PIM will provide a significant contribution to the development of high performance HT-PEMFC

Poster Presentation : **POLY.P-27**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthesis and Thin Film Properties of Novel Photo-patternable Polyimide Gate Insulator with Trimethylolpropane Triacrylate Crosslinker

So Eun Chun, Taek Ahn*

Department of Applied Chemistry, Kyungsung University, Korea

The photo-patternable polyimide (DOCDA-6FHAB-IEM) containing urethane linkages as side chains was successfully synthesized with a simple one-step methacrylate esterification of the hydroxyl group having soluble polyimide (DOCDA-6FHAB) and isocyanatoethyl methacrylate (IEM). DOCDA-6FHAB-IEM polymer was mixed with trimethylolpropane triacrylate (TMTA) as photo-crosslinking agent and Irgacure 184 as photo-initiator. We have confirmed the photo-crosslinking process through FT-IR measurement before and after UV-visible exposure to polymer film. Crosslinked DOCDA-6FHAB-IEM+TMTA film showed good surface roughness as root mean square (rms) value as about 0.240 nm in AFM measurement and the surface energy of crosslinked DOCDA-6FHAB-IEM+TMTA was also found to 46.37 dyne/cm. Detailed film fabrication condition and further electrical characterizations of thin film will be presented.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-28**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthesis and Characterization of Novel Photo-crosslinkable Polyimide Gate dielectric with the Bisphenol A Dimethacrylate Crosslinker

Jin A Park, Taek Ahn*

Department of Applied Chemistry, Kyungsung University, Korea

The soluble photo-crosslinkable polyimde having vinyl group (DOCDA-6FHAB-IEM) was prepared with methacrylate esterification from the reaction of hydroxyl group containing polyimde (DOCDA-6FHAB) and NCO group containing isocyanatoethyl methacrylate (IEM). And then, DOCDA-6FHAB-IEM polymer was mixed with bisphenol A dimethacrylate (Bis-DMA) as photo-crosslinking agent and Irgacure 184 as photo-initiator. The film was irradiated with UV-visible. We have confirmed the photo-crosslinking mechanism through the FT-IR measurement. Thin film properties of crosslinked DOCDA-6FHAB-IEM+Bis-DMA film were systematically characterized such as chemical structures, surface roughness, surface energy, thermal stability, dielectric constant and capacitance, etc. Detailed film fabrication condition and thin film properties will be presented.

Poster Presentation : **POLY.P-29**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Polymerization-induced microphase separation of Janus bottlebrush polymers to ordered nanostructured materials

Changsu Yoo, Myungeun Seo*

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

Polymerization-induced microphase separation (PIMS) has attracted significant attention due to its facile way of preparing nanostructured materials with tunable macroscopic shapes. In most previous PIMS, the incorporation of a cross-linker in the system captures the desired morphology before the order to disorder-transition. The resulting polymer has a robust and disordered bicontinuous structure so they are widely used in various applications like nanoporous polymer, polymer electrolyte, and anion exchange membrane. Nevertheless, the ordered structure like lamellae morphology is also important for nanolithography and nanowire arrays. However, the PIMS system without the crosslinker for ordered structure encounters the heterogeneous polymer and batch-to-batch difference result. Here, we investigate the effect of Janus bottlebrush polymer on PIMS behavior concerning the formation of ordered structures. A Janus bottlebrush polymer, one type of bottlebrush polymer, exhibits extended morphology due to steric hindrance between densely grafted side chains along the backbone. Especially, Janus bottlebrush polymer has different side chains on each repeating unit of backbone, showing an efficient and unique self-assembly behavior. By comparing the PIMS behaviors of two different architectures, we will discuss the important factors that determine the final nanostructure. The synthetic route and microphase separation behavior of linear and Janus bottlebrush PIMS will be presented in detail.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-30**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Kinetically captured ordered morphologies via polymerization-induced microphase separation by the high χ monomers

Wonjune Yeo, Myungeun Seo[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Polymerization-induced microphase separation (PIMS) is a versatile method to produce 3D bicontinuous nanostructure. Subsequent etching of a specific domain could make the 3D bicontinuous nanoporous materials which have huge potential for separation, catalyst support, adsorbent, etc. Although the properties of nanoporous materials have a close relation with the shape of the morphologies such as lamella, cylinder, and gyroid, the kinetic capture of phase during development of morphologies prevents access to the ordered morphologies. To overcome the kinetic issue and reach the ordered state, we introduced the high χ monomer which could facilitate the phase separation faster. The reversible addition–fragmentation chain transfer (RAFT) polymerization was used for the synthesis of block copolymers with or without the high χ monomer. Depending on the high χ monomer, we observed the kinetically captured ordered morphologies such as cylinder and lamella.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-31**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhanced Optical Response through Positional Variation in Self-Assembled Supramolecular Structures

Kangseok Kim, Jun Su Kang, Myungeun Seo*

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

Natural molecules that exhibit directional preference, such as amino acids and proteins, demonstrate efficient and systematic properties compared to synthesized polymers. Various attempts are being made to unveil the origin of homochirality in biomolecules like these. Among these efforts, extensive research is being conducted on self-assembled supramolecular structures. Supramolecular chirality possesses dynamic properties that change in response to external stimuli, and its distinct cooperative nature allows for the amplification of circular dichroism(CD) signals. Specifically, through the utilization of diacetylene-containing triphenylamine (DA-TPA), we achieved the manipulation of structural handedness through circularly polarized light (CPL), unveiling the mechanisms underlying this chiral transfer process. Nevertheless, understanding the relative positioning and connectivity between the TPA core and the diacetylene group remains limited. In this study, we aim to identify the factors of change within the self-assembly process resulting from the positional variation of diacetylene groups, presenting molecules that induce an enhanced optical response.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-32**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Development and synthesis of Anthracene based fluorescence for Aggregation-induced emission

Jieun Lee, Kim Hyerin, Yeong Soon Gal[1], Sung-Ho Jin[*]

Department of Chemical Education, Pusan National University, Korea

[1] *Department of Fire Safety, Kyungil University, Korea*

Highly efficient blue or deep-blue materials are important for full-color display and efficient white lighting OLEDs. Compared with red and green emitters, however, the blue emitter with high efficiency, color purity and long lifetimes still remains a huge challenge. Therefore, it is necessary to find a way to develop high efficiency, stable blue or deep-blue fluorescent materials. In this study we successfully synthesized (4-(10-(4-(9H-carbazol-9-yl)-2-methylphenyl)anthracen-9-yl)-3-methylphenyl) diphenylphosphine oxide (CZm-AN-mPO) through palladium-catalyzed Suzuki coupling reactions. In degassed THF solution, its emission exhibited a blue emission at 425nm with relatively narrow full width at half-maximum of less than 40nm, and CZm-AN-mPO showed a high photoluminescence quantum yield over 70% with a short decay lifetime of 2.31ns. Additionally, to investigate the aggregation-induced emission (AIE) properties, the PL emissions were measured in THF/water mixtures with different water fractions. The PL intensities were gradually reduced and slightly red-shifts by adding water into the THF solution due to decreased solubility and strong intermolecular π-π interactions in aggregated states. This result shows the AIE nature of CZm-AN-mPO.

Poster Presentation : **POLY.P-33**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Strengthen Block Copolymer Ion Gels Using Surface-Modified Aramid Nanofiber (S-ANF)

Seonwoo Yang, Taeseok Oh, Myungeun Seo*

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

Due to their low volatility, nonflammability, electrochemical stability, and high ionic conductivity, ionic liquids (IL) are utilized in various fields, such as electrochemical actuators, supercapacitors, or lithium ion batteries. However, as the name suggests, ILs are “liquid”, which means that it can flow, not maintaining its physical form. To utilize ILs in desired places, mechanical strength should be guaranteed. Block copolymer ion gel was reported with poly(styrene)-b-poly(ethyl acrylate)-b-poly(styrene) (SEAS), poly(styrene)- b-poly(methyl methacrylate)-b-poly(styrene) (SMS), and poly(styrene)-b- poly(ethylene oxide)-b-poly(styrene) (SOS). These gels showed enhanced mechanical strength and well-ordered microstructure, albeit lowered ionic conductivity. In our work, surface-modified aramid nanofiber (S-ANF) was utilized to enhance mechanical strength while maintaining high ion conductivity. Physical properties and electrochemical performances were examined with respect to S-ANF and block copolymer loading.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Characterization of various polymer networks prepared by catechol-based crosslinking

Minjeong Kang, Jungju Ryu[1], Daewon Sohn[*]

Department of Chemistry, Hanyang University, Korea

[1]*Department of Chemistry and Research Institute for Convergence of Basic Science, Hanyang University, Korea*

Catechol moieties have been attracted as bio-inspired glue observed in mussel byssal threads. The binding types vary through catechol oxidation and coordination bonds. In this presentation, we introduce catechol-based crosslinking methods using various polymers: hyaluronic acid, chitosan, and poly(ethylene glycol). In particular, the internal structures were compared among the three networks to understand the main factors that influence the network structures. The carboxylic acid groups on HA and chitosan were substituted, and the succinimidyl end groups of tetra-arm PEG were modified with dopa moieties. The polymer gels were prepared by pH controls with Fe(III) ions. The internal structures were examined using small-angle scattering measurements. The results demonstrated that the networks are governed by polymer conformation in the polyelectrolyte gels: HA and chitosan gels. On the other hand, it was observed that the crosslinking types influenced dominantly the structures of PEG gels consisting of neutral chains.

Poster Presentation : **POLY.P-35**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

Composite of onion extract-derived carbon dots with polyvinyl alcohol: Thin film preparation for UV light-blocking applications

Akshay S. Patil, Daewon Sohn[1,*]

Department of Chemistry , Hanyang University, India
[1]*Department of Chemistry, Hanyang University, Korea*

In this work, we synthesized carbon dots from onion extract (OE-CDs) by the hydrothermal method. Despite their small size, these carbon dots can absorb large amounts of UV light. The film was prepared using an OE-CDs composite with polyvinyl alcohol to block UV light. To check the size of synthesized carbon dots we used the TEM characterization technique. The particle size is around 94 nm. X-ray photoelectron spectroscopy reveals carbon, oxygen as well as nitrogen, and sulfur element and their atomic weight percentage present in OE-CDs. Synthesized carbon dots show a dual role in composite thin films, antibacterial as well as UV blocking. Due to the presence of the sulfur group in the carbon dot, the composite film showed antibacterial properties. The onion-derived carbon dots (OE_CDs) synthesized via a hydrothermal method, have successfully blocked the complete UV-C and UV-B regions (200 nm – 315 nm). From the UV-A region, in the wavelength range of 315 nm - 350 nm, 77% of UV light was absorbed.

Poster Presentation : **POLY.P-36**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Introduction of Pyrazine Based Polymer for Dopant Free Green Solvent Processed Hole Transfer Material in High Performance Perovskite Solar Cells

Jeonghyeon Park, Chetan Lakshman, Bo Hyeon Cho, Yeong Soon Gal[1], Sung-Ho Jin[*]

Department of Chemical Education, Pusan National University, Korea

[1]*Department of Fire Safety, Kyungil University, Korea*

The new Polymer is designed and synthesized for fabrication of perovskite solar cells (PSCs) application. Nap1-PzTBr used as dopant-free Green solvent processed hole transport material (HTM). The thermal, photophysical and electrochemical properties of Nap1-PzTBr were systematically investigated. Nap1-PzTBr exhibited a band gap of 1.96 eV with highest occupied molecular orbital (HOMO) of -5.596eV and Lowest unoccupied molecular orbital (LUMO) of -3.636eV. The electron withdrawing nature of pyrazine results in better intermolecular interactions, affording high hole mobility and charge transfer properties. Thus, optimized Nap1-PzTBr based device showed the power conversion efficiency of 21.2% with open-circuit voltage of 1.07V, a short-circuit current density of 25.07mA/cm2 and a fill factor of 78.96%. This result indicated that pyrazine based polymer have great to further development of HTM.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-37**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

RAFT-Mediated Syntheses of Stimuli-Responsive Block-copolymers for Metal-Chelated Nanocatalysts

Sang-Min Lee

Department of Chemistry, The Catholic University of Korea, Korea

We present the syntheses of poly[PEG methacrylate)]-b-[poly(methacrylic acid)-co-poly(N-isopropylacrylamide)], [pPEGMA-b-(pMAA-co-pNIPAAm)], through reversible addition-fragmentation chain transfer (RAFT) polymerization. pMAA, pPEGMA, and pNIPAAm are well-known stimuli-responsive polymers that are sensitive to pH and temperature, respectively. The resulting copolymers can form a core/shell-type self-assembled nanostructure by coordination-induced self-assembly in aqueous solution and can exibit the characteristic Lower Critical Solution Temperature (LCST), allowing for the stimuli-responsive control of catalytic reactions.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-38**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

The New Spiro-type Hole Transport Material in Non-Hazardous Solvent Process in Perovskite Solar Cells.

Donghyun Song, Zhiqing Xie, Yeong Soon Gal[1], Sung-Ho Jin[*]

Department of Chemical Education, Pusan National University, Korea

[1]*Department of Fire Safety, Kyungil University, Korea*

Perovskite solar cells (PSCs) are the fastest developing solar cells and pull in a part of attention due to the prevalent advantages such as solution process, flexibility, light weight and low cost. In common, Spiro-OMeTAD is the most using hole transport material (HTM) in PSCs. Thanks to its good merits, such as increasing molecular stability, forming smooth films, high tolerance with dopants, and matching energy levels with perovskite. Therefore, based on structure of Spiro-OMeTAD, Spiro-P was designed and synthesized by using end group engineering. The thermal, optical, electrochemical properties of the new HTM and device performance were investigated. As a result, Spiro-P based device showed high power conversion efficiency (PCE) of 22.36% with an open circuit voltage (Voc) of 1.102V, a short-circuit density (Jsc) of 26.20mA/cm2 and a fill factor (FF) of 77.43%. This investigation shows that the new synthesized Spiro-P is a potential HTM to achieve good performance in the field of PSCs.

Poster Presentation : **POLY.P-39**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Lanthanide-Chelated Hybrid Polyionic Complex of Zwitterionic Polymer Shell for Luminescent Nanoplatform

Jiye Choi, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

This study presents the synthesis of poly[(2-methacryloyloxyethyl phosphorylcholine)-b-(poly methacrylic acid)], p(MPC)-b-p(MAA), block-copolymers through reversible addition and fragmentation chain transfer (RAFT) polymerization. The resulting copolymers can form a core/shell-type self-assembled nanostructure by terbium chelation in aqueous solution. In addition, we present a comprehensive exploration of the optical properties of terbium-chelated nanoparticles through the conjugation of ligands.

Poster Presentation : **POLY.P-40**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Metal-chelated Hybrid Polyionic Complex of Multi-Agent Loading Capability by Coordination-Induced Self-Assembly

Eunseo Lee, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

We present the synthesis of poly[tert-butyl acrylate]-b-poly[PEG methacrylate], poly(tBA)-b-poly(PEGMA), through Atom Transfer Radical Polymerization (ATRP). After the deprotection of tert-butyl groups in poly(tBA) block, poly(acrylic acid) (PAA) was obtained for the electron-rich carboxylate functional groups that can easily coordinate versatile transition metal cations while poly(PEGMA) block provides an excellent biocompatibility. Using the metal-mediated self-assembly strategy, nanostructures encapsulating metal cations(Fe2+,Fe3+,Ni2+,Cu2+) can be prepared in a facile manner, which can then be employed as a delivery system for the biocatalytic agents. Additional organic compound or inorganic compound like hydrophobic drug can be loaded for each metal-enabled system.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Syntheses of Chemically Modifiable Amphiphilic Block-Copolymers for Facile Preparation of Functional Nano-Assemblies via Post-Synthetic Modification

Gyeong-Tae Wi, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

Core-shell nanoparticles made of poly(glycidyl methacrylate) (PGMA) and poly(methacrylic acid) PMAA and surrounded by a poly(ethylene glycol) methacrylate (PEGMA) shell are synthesized and characterized. Because PGMA has vinyl and epoxy groups, it can be used in bio applications by combining with biopolymers. We combine GMA with organic dyes to observe the efficacy of nanoparticles and apply metal chelation to PMAA to impart two multifunctional properties. It can be applied to various fields such as drug delivery, imaging diagnosis, and biosensors.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

RAFT-Mediated Synthesis of Zwitterionic Double-Hydrophilic Block-Copolymers for Core/Shell-Type Nanoassembly

Jiwoo Park, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

Poly(sulfobetaine methacrylate) (PSBMA) has been studied as a zwitterionic polymer that provides colloidal stability through its high hydrophilicity. Also, PSBMA has unique temperature-sensitive behavior with an upper critical solution temperature (UCST). In this study, the block-copolymer poly(sulfobetaine methacrylate)-b-poly(methacrylate) (PSBMA-b-PMAA) was synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization in aqueous solution. The PSBMA-b-PMAA can form core/shell-type self-assembled nanoparticles by chelating Cerium(III) as a redox-active center with methacrylate blocks. The resulting Cerium-chelated nanoparticles will exhibit great potential for biomimetic oxidation-reduction nanocatalysis in an aqueous solution.

Poster Presentation : **POLY.P-43**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Dithienobenzothiadiazole-Based Polymer Donor in All-Polymer Solar Cells with Phenyl-substituted Siloxane Terminal Groups

Priyanka Yadav, Yeong Soon Gal[1], Sung-Ho Jin[2,*]

Department of chemical materials, Pusan National University, India

[1]Department of Fire Safety, Kyungil University, Korea

[2]Department of Chemical Education, Pusan National University, Korea

Dithienobenzothiadiazole (DTBT) and benzodithiophene (BDT)-based wide band gap (WBG) polymer donors were investigated for use in all polymer solar cells. To further increase the solubility, blend miscibility and film morphology, a phenyl group substituted siloxane-based side chain was added to the BDT unit. New polymer Ph-Sil-1 was synthesized and carried out the characterizations systematically. Ph-Sil-1 showed film absorption peak at 380 nm and optical band gap of 2.20 eV. The complementary absorption and energy offsets were observed between Ph-Sil-D1, PM6 polymer donors and PY-IT acceptor. The PM6: Ph-Sil-1: PY-IT based All-PSCs resulted an open-circuit voltage of 0.93 V, a short-circuit current density of 25.4 mA cm−2, and a fill factor of 68.9%, corresponding to a power conversion efficiency (PCE) of 16.1%. The results emphasize that Ph-Sil-1 can be a powerful donor, which is favorable in the construction of simple WBG polymer donors for efficient All-PSCs.

Poster Presentation : **POLY.P-44**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Chemically Modified Polysaccharides for Facile Formation of Functional Single-Chain Nanoparticles

Yeonjoo Jung, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

Chitosan as a biocompatible natural polysaccharide has been investigated as a versatile polymeric scaffolds for systemic delivery platforms and local injection gels. However, many of such chitosan derivatives often suffer from low aqueous solubility and extremely high viscosity under a wide range of pH conditions, which significantly limits their wide applicability. Herein, the natural chitosan was non-enzymatically ligated with monosaccharides for the enhanced solubility at neutral pH, follow by the chemical modification with chelating agents that can be utilized as a multidentate ligand for versatile metal cations. The chelating agent can also bind to metals and at the same time create crosslinking bonds between the polymers to form nanoparticles. The resulting metal-chelating, glycated chitosan has been self-aggregated into nanoscale structures. These structures will be able to release reversible cargoes by external stimuli such as pH changes and create single-chain nanoparticles that form nanoparticles into a single chain of polymers at very dilute concentrations. Its properties and colloidal properties will be discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Monodisperse Cyclic Polymer Mechanochemistry

Gregory Peterson[*], **Kyoung Taek Kim**[1], **Tae-Lim Choi**[2]

Chemistry, Incheon National University, Korea
[1]*Division of Chemistry, Seoul National University, United States*
[2]*Department of Materials, ETH Zürich, Switzerland*

We studied the mechanochemical degradation of a series of monodisperse cyclic and linear poly(D,L-lactide)s (PLA). Polymers were subjected to ultrasonication (US) and ball-mill grinding (BMG) and their degradation kinetics and scission products were characterized. Cyclic polymers exhibited 9.0- and 1.9-times larger scission rates than linear PLA with US and BMG, respectively. Linear intermediate products from cyclic polymers were observed using BMG and US, although more sensitive techniques were required for US. Daughter fragment dispersity trends provided insight into a dynamic memory effect during US, which was not present with BMG. These results provide important insight into the influence of the cyclic polymer architecture in mechanochemical reactions.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Porphyin-based Covalent Organic Framework

Inyoung Bae, Woo-Dong Jang[*]

Department of Chemistry, Yonsei University, Korea

Porphyrin-based two-dimensional (2D) covalent organic frameworks (COFs) have been gain much interest in recent years due to their structual versatility and high stability. Most porphyrin-based COFs contain only one metal in the COF and deal with their efficiency as a catalyst in the fields such as CO_2 reduction reaction, hydrogen evolution, etc. However, the effect of the combination of metals on a building units, which should be benefical for their utilization, is still far-away explored. Herein, we conducted imine condensation reaction of 5,15-bis(4-formyl-phenyl)porphyrin$_{M1}$ (BFPP$_{M1}$, M1=H2, Ni, Cu, Zn) and 5,10,15,20-tetra(4-aminophenyl)porphyrin$_{M2}$ (TAPP$_{M2}$, M2=H2, Cu), leading to the formation of isostructural porphyrin-based covalent organic frameworks BFPP$_{M1}$-TAPP$_{M2}$-COF). Strutures of the resulting BFPP$_{M1}$-TAPP$_{M2}$-COFs were confirmed thouhgh FT-IR, PXRD and TEM. Since BFPP$_{M1}$-TAPP$_{M2}$-COFs with various metal combinations were synthesized, we plan to study photocatalytic activity depending on the metal combinations.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-47**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Thermoresponsive nanocellulose membrane for selective oil-water filtration.

Zubaida Hassan

Chemistry, Yonsei University, Korea

Most traditional filtering membranes are made of materials that are hard to recycle such as nylon, PVC, etc., and often have a fixed wettability; that is, they are either superhydrophobic (only wettable to oil) or superhydrophilic (only wettable to water). This leads to double their production and generating even more waste. This research makes a humble attempt at synthesizing an easily biodegradable membrane that showcases switchable wettability in response to an external stimulus. Here, an environment-friendly, thermoresponsive membrane of nanocellulose grafted with a high molecular weight amine-terminated poly(2-isopropyl-2)oxazoline was synthesized. The nanocellulose fibers were synthesized from pinewood scraps and were modified by TEMPO (2,2,6,6-Tetramethylpiperidine-1-oxyl) mediated oxidation to efficiently graft the poly(2-isopropyl-2)oxazoline via peptidic coupling reaction. The structures and the successful grafting of the two materials were evaluated by various characterization methods. The FT-IR, XRD, and FESEM scans show the step-by-step structure and morphology of nanocellulose synthesis as well as its further modification and subsequent grafting with poly(2-isopropyl-2)oxazoline polymer. The preliminary characterization of poly(2-isopropyl-2)oxazoline was conducted by GPC and was then finally characterized by H-NMR spectroscopy. The switchable hydrophilic to oleophilic behavior was characterized by temperature-controlled UV analysis, and a sharp change was reported near 50°C, which is in accordance with the LCST of the grafted polymer. Thus, a thermoresponsive colloidal nanocellulose suspension was successfully synthesized as a nanoremediation material.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **POLY.P-48**

Polymer Chemistry

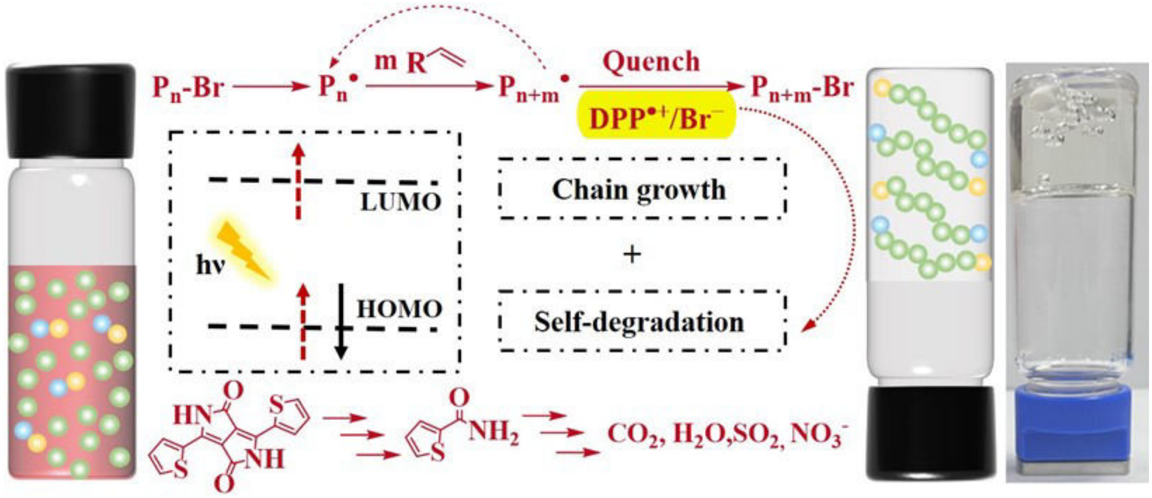
Exhibition Hall C FRI 11:00~13:00

Mediating the progress of organo-photocatalyst intermediate in ATRP to produce pure polymers with ultra-high molecular weight

Long Yang

Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

Photopolymerization, acting as photo-redox reaction, is growing to be one of the emerging and promising fields of solar-light utilization and chemical transformations as an appealing method for the synthesis of metal-free polymer materials with well-defined microstructures and architectures, due to the mild, environment-friendly and light-controlled three-dimensional processing. However, producing polymers in this way contains residues of photocatalysts (PCs), and the process of purification is still challenging, especially for the applications in electrics, biological tissues and human bodies. Although low-loading catalysts reduce the pollution of polymers, most PCs tend to introduce unknown color and toxicity to synthetic polymers and the application terminals. Herein, with diketopyrrolopyrrole (DPP) derivative photocatalysts we developed a technology of photo-ATRP program, which conducted the simultaneous catalyst self-degradation in the polymerization process of monomer initiation/chain growth, resulting in pure polymers without color and impurity residues. Blue light generated transparent polymer PMMA emerged as gel state with ultrahigh molecular weight (MW) of around 2,200,000 and a low dispersity of about 1.38, which held the highest MW and the great applying potential in light curing resins. This energy-saving polymerizing and light-controlled technique can expand the synthesis and application of resins without further purification and is expected to be applied in 3D photopolymerization.


P_n-Br
$P_n^{\bullet}$
m R
$P_{n+m}^{\bullet}$
Quench
$DPP^{\bullet+}/Br^-$
P_{n+m}-Br
LUMO
hv
HOMO
Chain growth
+
Self-degradation
HN
O
S
NH
NH_2
CO_2, H_2O,SO_2, NO_3^-

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Detection of TNT Vapors by Fluorescence Quenching Using Highly Fluorescent Conjugated Silole Polymers

Honglae Sohn[*], <u>Kyoungkuk Koh</u>

Department of Chemistry, Chosun University, Korea

This study presents the synthesis, characterization and evaluation of two new conjugated polymers for the detection of chemical explosives. The polymers, denoted as P1 and P2, exhibited significant responses to fluorescence quenching and photoluminescence (PL) recovery processes in the presence of TNT vapors. The unique photophysical properties of the polymers were attributed to their aggregation-induced emission (AIE) and intramolecular charge transfer (ICT) effects. The investigation of solvent behavior and ICT properties using density functional theory (DFT) calculations provided insights into the conjugated π□14 systems of the polymers. The fluorescence and sensing properties of P1 and P2 were studied in various states, including pure THF solution, films, and aggregated states. The quenching effects varied between the solution and solid states, highlighting the differences in sensitivity. However, both polymers exhibited high fluorescence efficiencies in all three states. Overall, these rigid polymers with strong fluorescence show promise as potential candidates for detecting explosives by improving the fluorescent properties of sensor films. The findings of this study contribute to the development of materials with enhanced detection capabilities for explosive compounds.This work was supported by the Technology Innovation Program (or Industrial Strategic technology development program, RS-2022-00154968)

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **POLY.P-50**

Polymer Chemistry

Exhibition Hall C FRI 11:00~13:00

Electronic Tuning of Iminotriphenolate Ligands for Titanium(IV)-catalyzed ROCOP of Cyclic Anhydrides and Epoxides

Seungyeon Jeong, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

This study investigated to development of an efficient Ti(IV) complex with iminophenolate ligands for alternating ring-opening copolymerization (ROCOP) of cyclic anhydrides and epoxides. ROCOP is a versatile synthetic method for preparing polyesters using relatively inexpensive and readily available monomers (epoxides and cyclic anhydrides). In comparison with flexible aminophenolate ligands, iminophenolate ligands are highly efficient for the preparation of Ti(IV)-based polymerization catalysts. Among the iminophenolate ligands, chloro-substituted ligand is the most effective and is more utilized to promote the Ti(IV)-catalyzed copolymerization of cyclic anhydrides (PA and NA) and epoxides (CHO, CPO, LO, and VCHO).

Poster Presentation : **POLY.P-51**
Polymer Chemistry
Exhibition Hall C FRI 11:00~13:00

One-step Wet-spinning of Conducting Polymer and Cellulose Nanofiber Composites for Fiber-Type Organic Electrochemical Transistors

Minhu Huang, **Myung-Han Yoon**[1,*]

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

In this study, we investigated the fabrication process and properties of composites based on poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) and cellulose nanofibers (CNFs) as active channel materials for fiber-type organic electrochemical transistors (OECTs). Utilizing highly crystalline, mechanically rigid, and chemically robust CNFs extracted directly from tunicates, we fabricated PEDOT:PSS-CNF composite fibers with varying concentrations of CNF (0, 5, 10, 20, and 30%) through a one-step wet-spinning process with a sulfuric acid-based coagulation medium. The inclusion of CNFs significantly enhances the mechanical strength of the composite fibers, achieving a Young's modulus of up to 16 GPa. Furthermore, fiber-type OECT devices based on an 80% PEDOT:PSS and 20% CNF composite exhibit the highest carrier mobility (4.0 $cm^2 V^{-1} s^{-1}$) with a marginal trade-off in volumetric capacitance (57 F/cm^3), resulting in an impressive benchmark performance parameter ($\mu \cdot C^*$) of 229 $F cm^{-1} V^{-1} s^{-1}$. Our findings suggest that the synergistic interaction between PEDOT:PSS and CNFs leads to a significant improvement in fiber properties, indicating that the resulting composite fibers have considerable potential for use in advanced wearable and textile electronics.

Poster Presentation : **IND.P-1**

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Interrelation between Surface Wettability and Orientation of Acrylic PSAs with Hydrophilicity Control for Medical Application

Ho Jun Song

Department of Advanced Materials Engineering, Korea Institute of Industrial Technology, Korea

Many drugs used in medical patches exhibit lipophilic properties, and therefore, many studies have been reported on non-polar hydrophobic acrylic PSAs However, polar hydrophilic materials are being developed with the development of the medical device industry, Accordingly, the necessity of hydrophilic PSAs is also gradually increasing. However, studies on hydrophilic PSA have not yet been conducted. In this study, we synthesize acrylic PSAs through photo-polymerization and controlled their hydrophilic properties using the content of a hydrophilic acrylate, 2-hydroxyethyl acrylate (HEA). In addition, Synthesized hydrophilic acrylic PSAs were investigated the change in morphology and rheology for the hydrophilic functional group on the properties according to the properties of polymer chains, chain orientation, and secondary bonding between chains. It also presented a simple method for evaluating affinity using the peel strength of hydrophilic acrylic PSAs and hydrophilic materials, polyvinyl alcohol (PVA) and hyaluronic acid (HA), and confirmed the potential for medical applications of hydrophilic acrylic PSAs through cytotoxicity and skin irritation test.

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Influence according to Functional Structure of Polysilsesquioxanes and POSS for Flexible Application

Ho Jun Song

Department of Advanced Materials Engineering, Korea Institute of Industrial Technology, Korea

With the development of flexible displays, various materials such as films, adhesives, and hard coatings require flexibility. In particular, hard coating materials for flexible displays need not only hard properties but also flexibility to protect flexible substrate. Silsesquioxane materials are attracting attention to realize such high performance properties. Silsesquioxanes have the formula RSiO1.5 (R is an organic group or H). Representative silsesquioxanes structure is polyhedral oligomeric silsesquioxane (POSS) of cage-like oligomer structure and the ladder-like polysilsesquioxane (LPSQ) structure. POSS and LPSQ show various differences in terms of structure and molecular weight. In this study, we analyzed the effect of the silsesquioxane structure on the mechanical properties by introducing cycloaliphatic functionalized POSS and LPSQ. As a result, the LPSQ-coated film showed a pencil hardness of 8H and high flexibility due to uniform coating properties.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Characterization of Crosslinking Network for PSQ/POSS Blended Films by UV Curing Process

Ho Jun Song

Department of Advanced Materials Engineering, Korea Institute of Industrial Technology, Korea

Recently, organic-inorganic hybrid materials have been widely used to overcome the disadvantages of organic polymers. Ladder-like polysilsesquioxane (LPSQ) and polyhedral oligomeric silsesquioxane (POSS) are representative organic-inorganic hybrid materials. The core of silsesquioxane is composed of Si-O-Si bonding. And the core is surrounded by organic side chains. Due to this unique structure, silsesquioxanes have a high interaction with the organic matrix, and is well soluble in organic solvents. Also, due to the Si-O-Si bonding of the core, it contributes to the improvement of thermal and mechanical properties. In this study, we introduced POSS into the LPSQ matrix to improve mechanical properties. Mechanical properties were analyzed using by pencil hardness and nanoindenter. When POSS was added, the pencil hardness and the hardness of the nanoindenter were increased.

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

One Pot Preparation of Spherical Magnesium Silicate by W/O/W Emulsion Precipitation Method

Kyeong-mun Jung, Youngyong Kim[1], Jaun An[2], Kyounghoon Lee[3,*], Ki-Young Kwon[2,*], ChanHo Jeong[4]

R&D department/Department of Chemistry, Denve.Inc/Gyeongsang National University, Korea

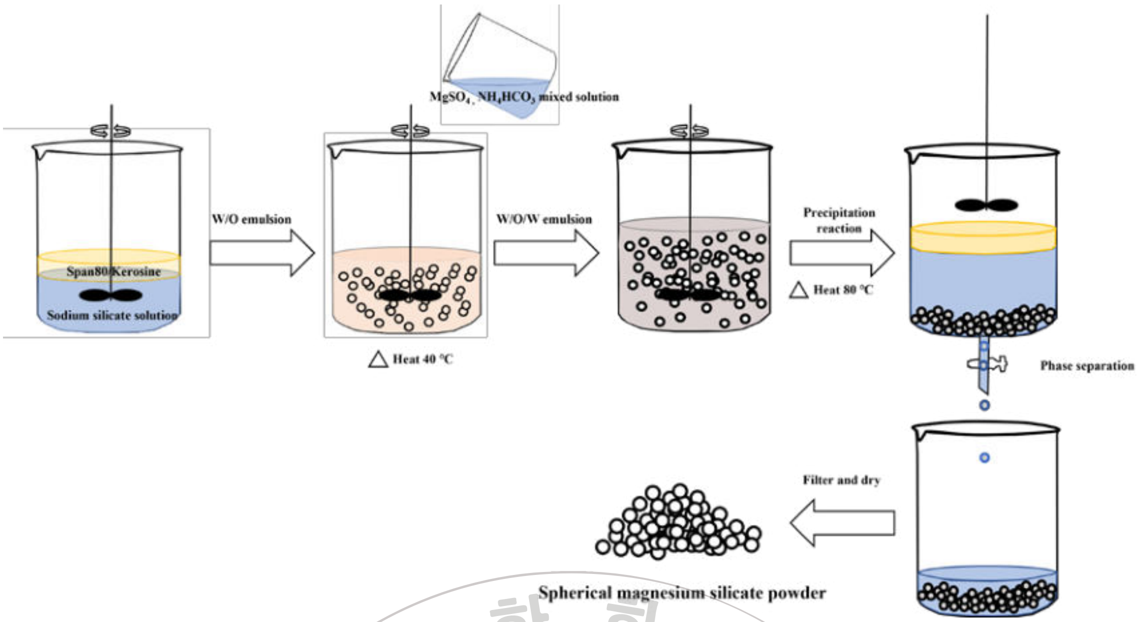
[1]*Department of Chemistry, Denve.INC, Korea*

[2]*Department of Chemistry, Gyeongsang National University, Korea*

[3]*Department of Chemical Education and Research Institute of Natural Sciences, Gyeongsang National University, Korea*

[4]*Department of Chemical education, Gyeongsang National University, Korea*

We report on the synthetic method of spherical magnesium silicate particles with a high specific surface area via a cost-effective water-in-oil-in-water (W/O/W) emulsification process. Notably, all samples of magnesium silicates prepared by this process exhibited specific surface areas ranging from 486.41 m^2/g to 662.23 m^2/g. In particular, the EM_2.81 sample showed approximately 1.5 times higher surface area than commercially used Magnesol XL. The high surface area originated from a high fraction of micropores. SEM analysis revealed distinct sections in the samples, indicating the optimal concentration of water glass for spherical shape maintenance. Additionally, most of the emulsion-treated EM samples displayed spherical morphology around 20 microns and demonstrated characteristics of excellent dispersion without aggregation in water. These results suggest that the W/O/W single-pot emulsification process is an effective method for producing magnesium silicate particles with high specific surface area and spherical morphology.


MgSO$_4$, NH$_4$HCO$_3$ mixed solution
Span80/Kerosine
Sodium silicate solution
W/O emulsion
Heat 40 °C
W/O/W emulsion
Precipitation reaction
Heat 80 °C
Phase separation
Filter and dry
Spherical magnesium silicate powder

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **IND.P-5**
Industrial Chemistry
Exhibition Hall C THU 11:00~13:00

A study on the manufacturing of TBHP used in chemical industry

Kim Cheolhyun

Dongsung Chemical Co., Ltd, Korea

Tert-butyl hydroperoxide(TBHP) is the main material used in the production of various organic peroxides. Furthermore, it is a kind of organic peroxide widely used as the initiator in (co)polymerization of styrene, butadiene, acrylonitrile and (meth)acrylates, the curing agent for vinylester resins and the high purity reagent in pharmaceutical and fine chemicals synthesis. Because it very easily forms radicals by external stimuli such as heat and light. Dongsung Chemical Co. Ltd. developed a technology to manufacture TBHP using TBA and hydrogen peroxide and commercialized it for the first time in Korea since 2022. In addition, we developed a technology to recover DTBP produced as a by-product through liquid/liquid extraction process. Detailed synthesis method and properties will be presented in the poster.This work was supported by the Industrial Cluster Program(www.kicox.or.kr)) funded by the Ministry of Trade, Industry and Energy(MOTIE, Korea). [Project Name: The localization of t-butyl hydroperoxide, a base material for organic peroxide used in polymerization / Project Number: PJN22007]

Poster Presentation : **IND.P-6**

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Development of a substance that simultaneously inhibits PVY and coronavirus

Seok Joon Lee*, **Sangtae Oh**[1]

College of Medicine, Pharmacology, Catholic Kwandong University, Korea

[1]*College of Medicine, Basic Sciences, Catholic Kwandong University, Korea*

Recently, considering the situation such as the Covid pandemic, it is very important and urgent to develop various antiviral drugs in order to prepare for the coming risks in advance. The most effective way to achieve that goal is to test natural products and their analogues. In the process, we discovered that a specific substance inhibits both PVY and the corona virus at the same time. To make this material commercially available, we have developed a synthetic method that is stereoselective and free of toxic reactants. In this presentation, we would like to present the synthesis method of the candidate material, and the inhibitory effect of PVY and coronavirus.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Bulk Etch Study for Monitoring of Pollution in Wafer

Sujin Kang, Jungi Lee, Dong Wook You*, Kwangshin Lim[1,*]

Process Technology Team, NvisANA, Korea
[1] *Research Institute, NvisANA, Korea*

The semiconductor manufacturing process is undergoing a trend of miniaturizing circuit features such as line widths and thinning gate oxide layers. As the demand for semiconductors increases, the importance of production yield becomes even more crucial. However, The increasing trend of high integration has resulted in chemical composition and molecular impurities exerting a more detrimental impact on the performance and yield of semiconductor components. This has led to a demand for higher precision in various measurement, analysis, and inspection processes. Particularly, the control of contamination on the wafer surface is considered an extremely significant challenge, and recently, inspection of metal contamination within wafers has also become a requirement. Bulk etching process is a technique used to uniformly remove the wafer surface to a specific depth in order to detect potential metal contamination within the wafer. In this study, the precise control of the reaction between HF and O3 is utilized to accurately manage the etch rate of the wafer and achieve uniform etch depths. The research results indicate that, with meticulous control, an etch depth of 1μm was targeted, resulting in an average etch depth of 1.07μm with a relative standard deviation of 4.44%. Furthermore, the proportional relationship between the supply times of HF+O3 and the etch depth was verified.

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Design and construction of a homebuilt solid-state NMR probes

Minseon Kim, **Yongae Kim**[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

In the case of solid-state NMR, a wide variety of sample states such as solid-state materials, crystalline materials, amorphous powders, and gel-state materials can be measured in solid-state NMR. Materials that can be measured by solid-state NMR can measure materials such as polymers or liquid crystals, biomolecules like proteins, nucleic acids. Probes used in existing commercialized NMR systems can perform various experiments, but probes can be made and used for specific research purposes or characteristics of samples. Such a homebuilt solid-state NMR probe may have a form and function more suitable for the purpose of the experiment and has the advantage of being able to be built at a low cost. In our laboratory, solid-state NMR probes were designed, manufactured, and used in-house according to the purpose of research for various samples. In particular, in the case of structural studies of biological samples such as membrane proteins, an environment similar to nature, such as lipid bilayer or bicelle samples, should be provided. Here, the composition of the homebuilt solid-state NMR probe and various 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, are introduced.

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

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

Development of filed-adaptive conductive plastic electrode system for reducing toxic microalgae

Jong Won Shin

Division of Daegu, Korea Institute of Science and Technology Information, Korea

Globally, the occurrence of toxic microalgae has led to ecological disruptions, mass mortality of livestock/wildlife due to toxins, mass mortality of farmed fish in aquaculture, significant economic losses due to water scarcity for various purposes, and a range of issues. Electrode plates used in water electrolysis can be made from various metals that utilize their ionization tendencies. Among them, electrode plates coated with platinum on materials like nickel alloys or titanium are known to exhibit excellent electrolysis performance.However, the manufacturing process of electrodes, including alloying and coating, requires additional processing steps, which can impact the production time and cost. Moreover, due to the metal manufacturing process, creating electrodes in various structures presents challenges.To address these challenges, we aim to develop a system utilizing polymer conductive plastics based on carbon composite materials for water electrolysis. This system will allow the electrolysis of water. Furthermore, we plan to apply this system to combat the proliferation of toxic microalgae.

Poster Presentation : **IND.P-10**

Industrial Chemistry

Exhibition Hall C THU 11:00~13:00

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

Ramesh Poonchi Sivasankaran

Environmental and climate technology, Post-doctoral researcher, Korea

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.1 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.2 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.3 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.4 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 : **INOR.P-11**

Inorganic Chemistry

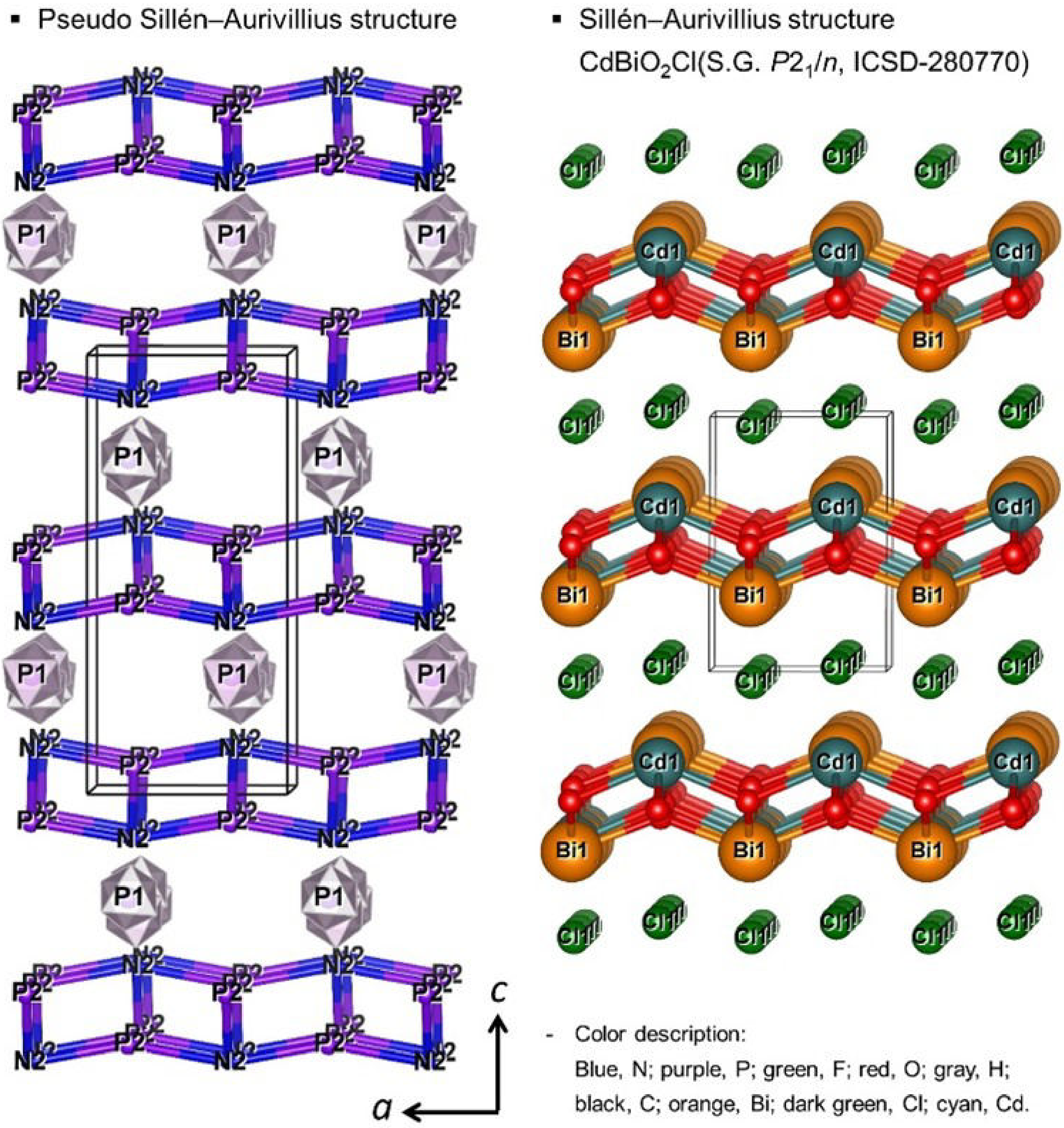
Exhibition Hall C THU 11:00~13:00

Novel Homochiral Metal-Free Pseudo Sillén-Aurivillius Perovskite

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Lead-based perovskite materials, particularly $MAPbI_3$ (MA: methyl ammonium), have garnered significant interest across various fields due to their promising properties. These materials hold great potential for applications; however, the predominant challenge lies in the toxicity associated with most lead halide perovskites. Overcoming this toxicity issue is crucial to fully harness their benefits and ensure their safe use in the future. Herein, we successfully synthesized metal-free perovskite by slow evaporation methods. The crystal structures of the title compound were determined by using single crystal X-ray diffraction (SC-XRD). SC-XRD results indicate that the title compounds crystallized in the orthorhombic chiral space group, $P2_12_12_1$(no. 19), attributed to the presence of chiral organic molecules. The title compounds reveal a zero-dimensional (0D) structure composed of ammonium cations, chiral organic cations, and hexafluorophosphate anions. Interestingly, considering hydrogen bond interactions, the overall structure of the title compounds extends to a pseudo three-dimensional (3D) structure with aurivillius layers. In this presentation, we present the synthesis, crystal structures, and properties of the novel metal-free perovskite, along with density functional theory (DFT) calculations.



- Pseudo Sillén–Aurivillius structure

- Sillén–Aurivillius structure CdBiO$_2$Cl(S.G. *P*2$_1$/*n*, ICSD-280770)

- Color description:
Blue, N; purple, P; green, F; red, O; gray, H; black, C; orange, Bi; dark green, Cl; cyan, Cd.

Poster Presentation : **INOR.P-12**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Polymerization of *rac*-lactide with Complexes [$L_{TH}MX_2$] (M = Zn, Pd; X = Br, Cl and L_{TH} = *(E)*-N^1,N^2-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine) and [LiO^iPr]

<u>Nguyen thi xuan Nhi</u>, Hyosun Lee[1,*]

Chemistry, Kyungpook National University, Korea

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

We have synthesized a series of complexes of Zn(II) and Pd(II), [$L_{TH}MX_2$] (M = Zn, Pd; X = Br, Cl) supported by the *(E)*-N^1,N^2-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine (L_{TH}). All complexes were characterized by ^{1}H NMR, ^{13}C NMR, elemental analysis (EA), and IR. X-ray single crystal diffraction revealed a distorted tetrahedral geometry for Zn(II) complexes, and a distorted square planar for Pd(II) complexes. Catalytic activity of these complexes with promotor LiO^iPr towards the polymerization of *rac*-lactide (*rac*-LA) were investigated at 0°C and 25°C. Specifically, it was shown that all complexes can effectively catalyze the ring-opening polymerization (ROP) reaction of *rac*-LA with more than 95% conversion within 20 minutes.

Poster Presentation : **INOR.P-13**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Insighting the Inhibitory Potential of Some 3d Metal Complexes Supported with Pyridine Derived *N,N,N*-Tridentate Ligand: Synthesis, Structural Properties, and Biological Evaluation

Saira Nayab, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

Transition metal complexes are being studied for their potential use in the development of metal-based drugs. Particularly, complexes comprising nitrogen bearing ligands with heterocyclic moieties have gained attention due to their ability to bind multiple biological targets. We presented pyridine-derived *N,N,N*-tridentate ligand, where **DEP-R** is *N^{1+}1,N^{2+}-diethyl-N^{2+}-(pyridin-2-ylmethyl)ethane-1,2-diamine*, in the synthesis of **[DEP-R(M)Cl_2**] (M = Fe, Co, Cu, and Zn) complexes. X-ray diffraction study revealed distorted trigonal bipyramidal geometry for the studied complexes. The ligand and its corresponding M(II) complexes exhibited superior bactericidal, fungicidal and leishmanicidal potential. Complexes also exhibited significant anti-urease potential against *Jack bean urease* (JB urease) and *Bacillus pasteurii urease* (BP urease). **[DEP-R($CoBr_2$)]**, exhibited considerable inhibitory potential against JB urease ($IC_{50} = 4.51 \pm 0.13$ μM) and BP urease ($IC_{50} = 5.71 \pm 0.14$ μM) relative to the standard thiourea (IC_{50} = 11.0 ± 0.62 and 9.10 ± 0.73 μM, respectively). To examine the structure-activity relationship, the complexes were docked at the active site of the respective protein and the results supported the experimental findings.

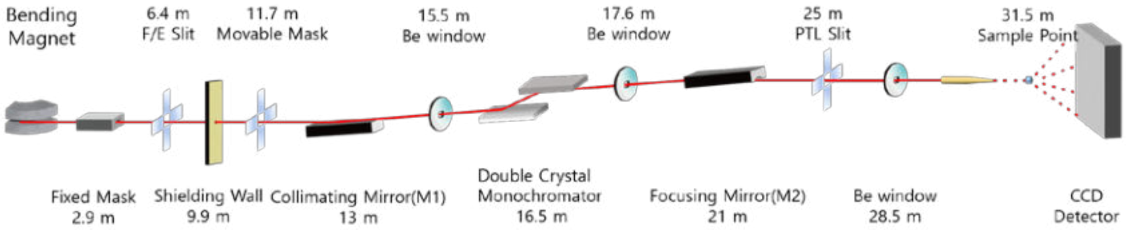
Poster Presentation : **INOR.P-14**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Overview of supramolecular crystallography Beamline and Software at Pohang Light Source II

Dae-Woong Kim, Jong Won Shin[1], Dohyun Moon*

Beam Operation Team, Pohang Accelerator Laboratory, Korea
[1]*Division of Daegu, Korea Institute of Science and Technology Information, Korea*

The beamline is located at the 2D bending magnet port within the 3 GeV storage ring of the Pohang Light Source II. It includes two mirrors (a collimating mirror and a focusing mirror) as well as a double-crystal monochromator (DCM) to deliver a photon flux of 6.2×10^11 photons per second. This photon flux is then focused to a focal point measuring 100 µm (horizontal) × 85 µm (vertical) at full width half maximum (FWHM) in the end-station. The beamline is designed for high-speed experiments and is equipped with a Rayonix MX225HS CCD detector and 10G network systems. Additionally, it supports temperature-dependent experiments spanning from 85K to 500K through the utilization of cryojet 5 equipment. Moreover, researchers have access to gas adsorption experiments and various optical experimental devices. This presentation will introduce the available instruments, provide an overview of the current status, and showcase the diverse range of applications facilitated by the utilization of the BL2D beamline.



Poster Presentation : **INOR.P-15**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

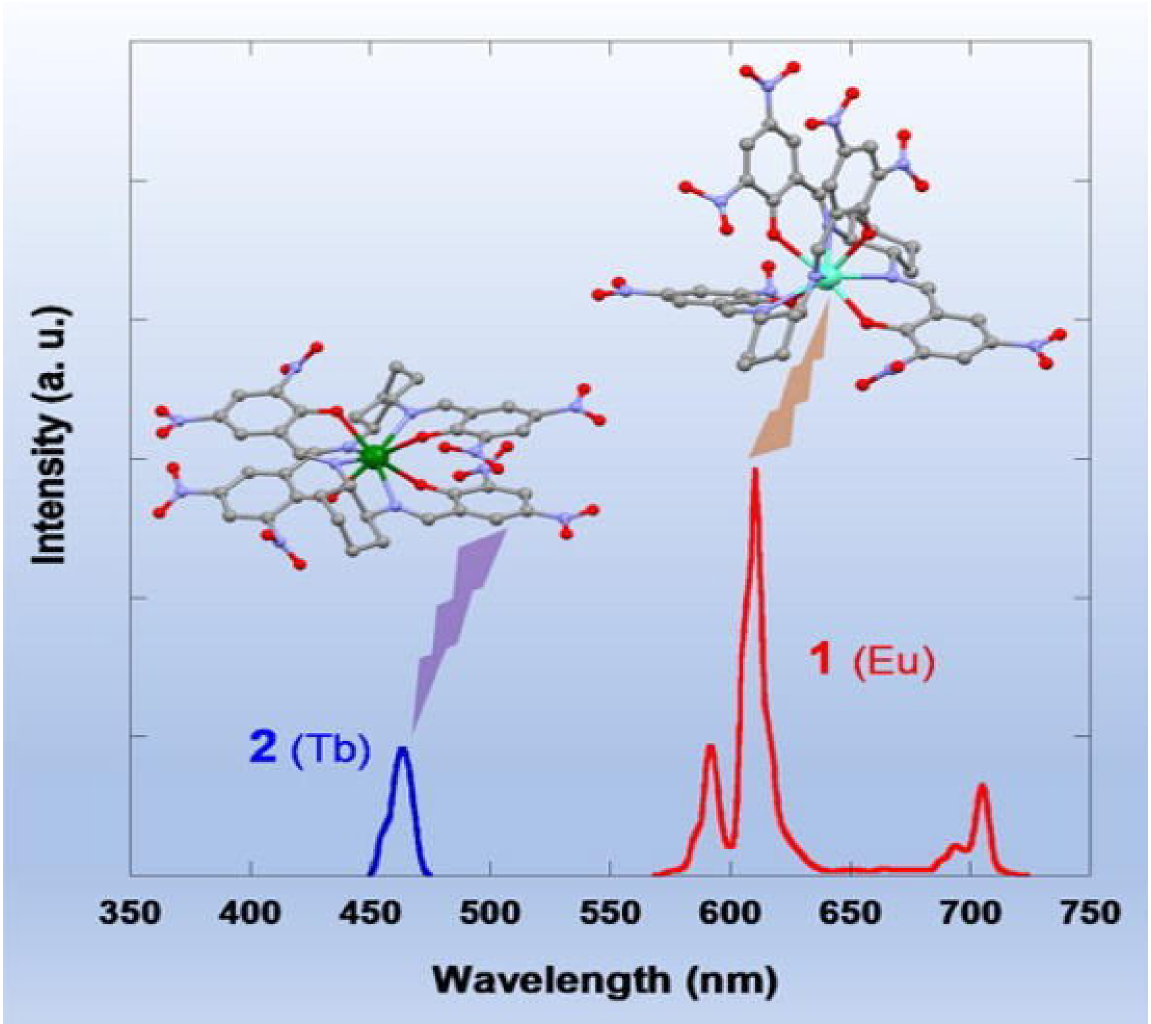
Synthesis, crystal structure, luminescence, and magnetic properties of lanthanide(Ⅲ) complexes containing chiral (S,S/R,R)-N,N'-bis(3,5-dinitrosalicylidene)-1,2-cyclohexanediamine ligand

Yuri Jeong, Anh Le Ngoc Tram[1], Ihsan Ullah[2], Bae Hyemin[3], Yoon Jung Jang[4], Kil Sik Min[*]

Department of Chemistry Education, Kyungpook National University, Korea
[1]*Chemistry, Kyungpook National University, Korea*
[2]*Department of Chemistry, Kuyngpook National University, Korea*
[3]*Department of chemistry education, Kyungpook National University, Korea*
[4]*College of Basic Education, Yeungnam University, Korea*

Molecular lanthanide complexes have attracted much attention in modern coordination chemistry because of their functional applications based on long-lived luminescence and magnetic properties. However, lanthanide metal ions that undergo f-f transitions are known to only weakly absorb UV/Vis light, and thus, appropriate ligand design is necessary to overcome this issue and achieve light emission by the antenna effect. In this research, enantiomeric mononuclear complexes (teaH)[Ln((S,S)-dnsalcd)2] and (teaH)[Ln((R,R)-dnsalcd)2] (Ln = Eu3+ for 1 and 4, Tb3+ for 2 and 5, and Sm3+ for 3 and 6), where teaH = triethylammonium and (S,S/R,R)-H2dnsalcd = (S,S/R,R)-N,N'-bis(3,5-dinitrosalicylidene)-1,2-cyclohexanediamine, were prepared and structurally characterized. The lanthanide(Ⅲ) ions of 1-6 were coordinated by four oxygen and four nitrogen atoms of two dnsalcd2- ligands and teaH+ was included as cation for charge balance. 1 and 3 were found to be isomorphous, and they exhibited a single intramolecular π-π interaction between two dnsalcd2- ligands. In contrast, 2 and 5 were found to be isomorphous, and they displayed two intramolecular π-π interactions between two dnsalcd2- ligands. Interestingly, complexes 1, 3, 4, and 6 showed strong Eu3+/Sm3+-based emissions, which were attributed

to the efficient antenna effects of the coordinated ligands. In contrast, 2 and 5 exhibited only weak ligand-based emissions. Finally, DFT calculations showed that 2 exhibited full delocalization via π-π interactions in the highest occupied molecular orbital (HOMO), whereas 1 contained a single localized benzene group in the HOMO, regardless of the presence of π-π interaction. In this presentation, we will describe the detailed preparation, structure, magnetism, and photoluminescence properties.



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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Chiral amino acid-templated Tin fluorides with lone pair stereochemical activity

Ahyung Jung, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Two types of new chiral amino acid-templated Tin fluoride crystals, (*R*)-Sn(IV), (*S*)-Sn(IV), (*R*)-Sn(II), and (*S*)-Sn(II), have been successfully synthesized via a slow evaporation method. The structures of Sn(IV)-compounds crystallize in the noncentrosymmetric nonpolar space group, $P2_12_12$. The structures of Sn(II)-compounds crystallizing in the polar space group, $P2_1$ were determined by single crystal X-ray diffraction. Interestingly, Sn(IV)-compounds exhibit a larger birefringence (0.289@1064 nm) attributed to the well-stacked arrangement of the planar π-conjugated benzene rings along the *b*-axis. Since tin(IV) fluorides can form more hydrogen bonds with ligands, the probability of π-π interactions between benzene rings increases and Sn(IV)-compounds can grow to centimeter-sized crystals easily. On the other hand, Sn(II)-compounds (0.85 × KDP) possess a stronger SHG response than Sn(IV)-compounds (0.46 × KDP) because of increasing the dipole moments due to the presence of the lone pairs. Besides, Sn(II)-compounds have photoluminescent properties due to the transition from the metal-to-ligand charge transfer (MLCT) contributed by the presence of the lone pairs.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Terbium(III) octanuclear complex based on tetradentate reduced Schiff base ligand: Synthesis, crystal structure, and magnetism

Anh Le Ngoc Tram, Yuri Jeong[1], Ihsan Ullah[2], Bae Hyemin[3], Yoon Jung Jang[4], Kil Sik Min[5,*]

Chemistry, Kyungpook National University, Korea
[1]*Kyungpook National University, Korea*
[2]*Department of Chemistry, Kuyngpook National University, Korea*
[3]*Department of chemistry education, Kyungpook National University, Korea*
[4]*College of Basic Education, Yeungnam University, Korea*
[5]*Department of Chemistry Education, Kyungpook National University, Korea*

Due to the distinct photoluminescence and molecular magnetism of lanthanide ions, the coordination chemistry of the ions has recently been growing as an interesting research area [1]. Luminescent lanthanide complexes are extremely useful in various optical applications, including tunable lasers, plastic optical fiber amplifiers, multicolor displays, and organic light-emitting diodes, thanks to their special photophysical properties [2]. Terbium(III) ion was selected for this research due to its reliably emitting green light with high color purity in both solid state and solution. The green emission holds significance in applications such as safety exit signals and security tags. Notably, substantial advancements have been achieved in the realm of green light-emitting electrochemical cells, contributing to the progress of this technology [3]. In this study, the synthesis of a new octanuclear lanthanide $Tb_8(C_{21}H_{28}N_2O_4)_4(OH)_8(NO_3)_8$ has been achieved using Tb(III) nitrate salt and a reduced Schiff base ligand (H_2L = [(2,2-dimethyl-1,3-propanediyl)bis(iminomethylene)bis(6-methoxyphenol)]). The composition of the complex was confirmed by elemental analysis, and its crystal structure was determined by single-crystal X-ray diffraction. The crystal structure revealed that the octanuclear compound crystallizes in the orthorhombic space group *Pbcn*. The structure has one Tb(III) ion located in the inner N_2O_2 compartment of the ligand, around by two nitrate anions coordinated. Besides that, two other Tb(III) ions are located in the distorted outer $O_2O_{2'}$ compartment of the reduced Schiff base ligand and coordinated by a hydroxyl bridge. Moreover, the three Tb(III) ions are connected through a hydroxyl ligand. Consequently, the structure of the octanuclear complex represents four corner-shared incomplete cuboidal $\{Tb_3O_4\}$ cores decorated with eight terminal nitrato, eight methoxy, and eight phenolato ligands. The complex was further characterized by FT-IR, UV-Vis, PL, and magnetism, providing valuable insights into its coordination chemistry. In photoluminescence, the octanuclear complex exhibits strong fluorescence in the 488–620 nm range. Furthermore, we have investigated magnetic properties with AC susceptibilities for SMM. In this presentation, we will describe the synthesis, structure, photoluminescence, and molecular magnetism in detail. References: 1. Xiao-Zhen Li, Chong-Bin Tian, and Qing-Fu Sun, *Chem. Rev.*, 2022, 122, 6374–6458.2. Zhuo Wang, Lizhen He, Bingqing Liu, Li-Peng Zhou, Li-Xuan Cai, Shao-Jun Hu, Xiao-Zhen Li, Zhikai Li, Tianfeng Chen, Xiaopeng Li, and Qing-Fu Sun, *J. Am. Chem. Soc.*, 2020, 142, 16409–16419.3. Guillaume Bousrez, Olivier Renier, Veronica Paterlini, Volodymyr Smetana, and Anja-Verena Mudring, *Inorg. Chem.*, 2021, 60, 17487–17497.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis, characterization, and dye adsorption of novel Cd-based coordination polymers

JinSoo Koh, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Two Cd-based coordination polymers, Cd(*S*) and Cd(*R*), have been successfully synthesized via hydrothermal reaction with the aid of chiral organic ligands. Single crystal X-ray diffraction (SC-XRD) reveals that both Cd(*S*) and Cd(*R*) crystallize in the monoclinic noncentrosymmetric (NCS) polar space group, $P2_1$ (No. 4). The asymmetric unit of the structure consists of two cadmium, two chiral ligands, two 2,2'-bipyridine molecules, and lattice water. Cd(*S*) and Cd(*R*) extend into 1D chains connected by π-π stacking interactions between chiral ligands and 2,2'-bipyridines, and T-shaped C-H…π interactions between 2,2'-bipyridines and hydrogen atoms of chiral ligand's phenyl rings. The title compounds exhibit a second harmonic generation (SHG) response of *ca.* 0.1 × KDP and are type-I phase-matchable. Interestingly, the title compounds possess good adsorption capacity for Congo red among various organic dyes. The maximum adsorption capacity of Cd(*S*) and Cd(*R*) was calculated through dye adsorption experiments at 850.82 and 817.71 mg/g, respectively.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Harnessing Plasmonic Effects for Efficient Upconversion in Y_2SiO_5:Pr^{3+} with $AgAu_3@SiO_2$

Hieu minh Ngo, **Kang Min Ok**[1,*]

Chemistry, Sogang University, Korea

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

We present a novel method to enhance the up-conversion efficiency of Y_2SiO_5:Pr^{3+}, a phosphor that emits UV light (280-340 nm) under visible light excitation. The conventional method of adding plasmonic particles to up-conversion nanomaterials suffers from quenching effects that reduce the emission intensity. To overcome this problem, we fabricated hollow shell Y_2SiO_5-coated particles with different shell thicknesses (70 nm, 116 nm, 177 nm, and 200 nm) by varying the amount of tetraethyl orthosilicate. We found that the optimal shell thickness was 177 nm, which resulted in the highest emission intensity among the samples. The SiO_2 layer played a dual role in enhancing the up-conversion efficiency: it increased the Y_2SiO_5 content during the annealing process and acted as a spacer between the plasmonic particles and the up-conversion nanoparticles, preventing quenching. By combining Y_2SiO_5 with $AgAu_3@SiO_2$ nanoparticles, we achieved a significant improvement in the up-conversion efficiency of Y_2SiO_5:Pr^{3+} without compromising its emission quality. This method offers a promising way to optimize the performance of plasmonic-enhanced up-conversion nanomaterials.

Poster Presentation : **INOR.P-20**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Tailoring 0D Optically Anisotropic Bismuth Halides Enabled by Superb Dual-ions Cosubstitution Engineering

Zhiyong Bai, **Kang Min Ok**[1,*]

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

Recently, lone pair cations have emerged as a class of efficient optically active units (OAUs) for designing birefringent crystals. However, compared to other lone pair cations such as $5s^2$ Sn^{2+} and Sb^{3+}, Bi^{3+} is received less attention as such OAUs probably attributable to its less stereochemically active $6s^2$ lone pair electrons. Against this background, introducing other type OAUs to Bi-based compounds might be a possible route for addressing the dilemma. Driven by this idea, in present study, we designed two 0D optically anisotropic bismuth halides. The first compound $Gu_3Bi_2NO_3Cl_8$ was obtained by implementing a superb dual-ions cosubstitution strategy from 2D perovskite halide $Cs_3Bi_2Cl_9$ with small birefringence. As expected, $Gu_3Bi_2NO_3Cl_8$ achieved a more than one order of magnitude birefringence enhancement (0.156 *vs.* 0.011) attributable to the replacement of spherical Cs^+ and Cl^- with strongly anisotropic $[C(NH_2)_3]^+$ and $[NO_3]^-$ moieties. The second compound $Gu_2Bi(NO_3)_3Cl_2$ was obtained by further replacing the Cl^- with more $[NO_3]^-$ anions (3.40-fold increase in number density) and thus this crystal exhibits a further improved birefringence of 0.177 at 546 nm.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Design an SBBO-type Metal Free Compound with Large Bandgap and Birefringence

Yang Li, Kang Min Ok[1,*]

Chemistry, Sogang University, China

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

Birefringent materials can modulate the polarization of light and thus have been widely applied in many advanced optical fields such as polarizing filters, optical waveplates, microscopy, and material analysis. Currently, in the deep-ultraviolet (DUV) wavelength region, only two birefringent materials, namely, MgF_2 and α-BaB_2O_4 have been commercialized. However, their limitation prompted researchers to investigate new DUV birefringent materials and the underlying mechanisms that could balance large birefringence and short UV cutoff edge.As a DUV birefringent material, there are some requirements that should be met simultaneously, including short UV cutoff edge (0.1 @1064 nm), and ease of large crystal growth. To satisfy the first two requirements, the functional building blocks (FBBs) possessing large HOMO-LUMO gaps and large polarizability anisotropy (Δα) are preferred such as $[C(NH_2)_3]$ (GU). Herein $Sr_2B_2Be_2O_7$ (SBBO) was selected as a template and GC was designed and grown via the slow evaporation method.As expected, GC features a pseudo-layer structure and overcomes the “stacking faults” of SBBO.GC exhibits a short cutoff edge (

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

Inorganic Chemistry

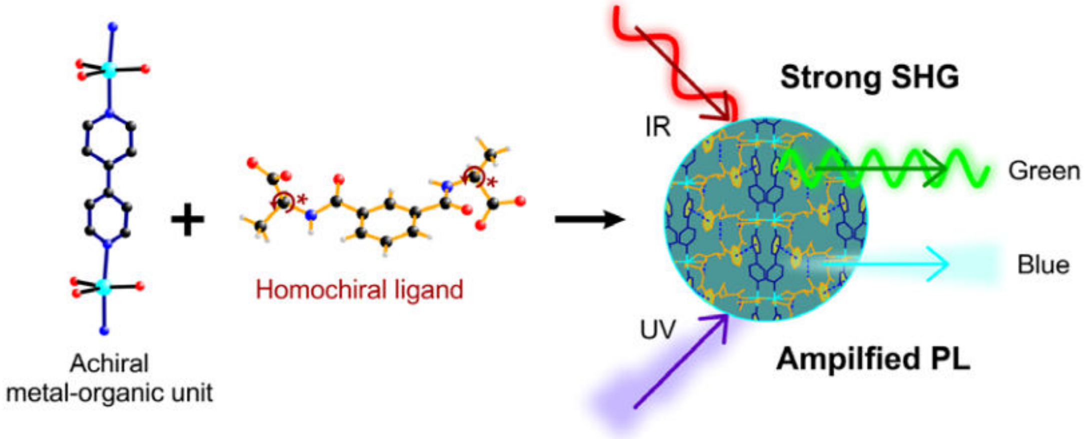
Exhibition Hall C THU 11:00~13:00

Homochiral d^{10}-metal coordination polymers with strong second-harmonic generation and amplified photoluminescence by excitation wavelength

Jihyun Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Homochiral coordination polymers (HCPs), a class of crystalline materials featuring chiral centers or helical arrangements, offer a distinctive advantage in design flexibility driven by the coordination of metal cations and chiral ligands. Among these, d^{10}-metal based HCPs emerge as promising candidates for optical materials due to their versatile structures, stability, and polarizability. The absence of an inversion center in the crystal structures places them within noncentrosymmetric (NCS) crystal classes, potentially leading to desirable energy-conversion phenomena, such as Second-harmonic generation (SHG). Despite the industrial interest in SHG-active crystalline materials, there is a limited number of reported candidates, indicating a promising research for further exploration.Herein, a new series of HCPs were synthesized by utilizing d^{10}-metal cations, alanine-based dicarboxylic ligands, and π-conjugated bipyridine ligand. For instance, compound 1 crystallizes in triclinic chiral space group, $P1$, as determined by single-crystal X-ray diffraction. Due to the unique three-dimensional structure with various functional groups in the ligands, compound 1 exhibits strong phase-matched SHG and reveals amplified photoluminescence (PL) emission upon excitation wavelengths. This presentation will cover the synthesis, structure determination, and optical properties of these HCPs.


Achiral
metal-organic unit
Homochiral ligand
IR
Strong SHG
Green
Blue
UV
Ampilfied PL

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Triptycene-Fused Asymmetric Multi-Resonance TADF Emitters and Their Photophysical Properties

Seung Hui Han, Hanif Mubarok[1], Rafi Muhammad Lutfi[2], Min Hyung Lee[1,*]

department of chemistry, University of Ulsan, Korea

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

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

Multi-resonance induced thermally activated delayed fluorescence (MR-TADF) emitters based on boron and nitrogen atoms have recently attracted great attention as highly efficient emitters in organic light-emitting diodes (OLEDs). We have recently reported a novel sterically shielded yet extremely rigid emitter, Tp-DABNA, in which the 3-D shape of triptycene (Tp) was successfully fused into the *B,N* core of the MR framework. Tp-DABNA exhibited a deep blue emission, high photoluminescence quantum yield (PLQY), a narrow full width at half maximum (FWHM), and reduced Dexter energy transfer (DET), ultimately leading to improved device efficiency. In this study, we prepared and characterized a series of Tp-fused asymmetric DABNA compounds comprising a Tp group and different *N*-arylated functional groups (1–6) to systematically control the photophysical properties, while leveraging the advantages of the Tp group. These compounds exhibited deep blue to sky blue emissions (λ_{PL} = 456–477 nm) in toluene solution and their TADF characteristics, such as emission color, FWHM, and delayed fluorescence lifetime, were fine-tuned depending on the employed *N*-aryl groups. We will discuss the details of synthesis, characterization, and photophysical properties.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Blue Fluorescence Compounds Based on Planarized B,N-Diarylated Benzonaphthoazaborine Ring

<u>Sae Bhin Cho</u>, Nhi Nguyen Ngoc Tuyet[1], Thi Quyen Tran[1], Taehwan Lee[2], Jaehoon Jung[1], Min Hyung Lee[1,*]

department of chemistry, University of Ulsan, Korea

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

[2]*chemistry, University of Ulsan, Korea*

Blue fluorescence compounds that exhibit high photoluminescence quantum yield (PLQY) and high color purity have attracted significant interest as the emitters in optoelectronic applications, such as organic light-emitting diodes. For this purpose, herein, a series of blue emissive, planarized B,N-diarylated benzonaphthoazaborine compounds (1~5), where electron-donating t-Bu and Me groups were introduced into the B-Ph, N-Ph, or benzoazaborine rings has been prepared and characterized. All compounds exhibited blue to sky-blue emissions (472–478 nm), which were significantly red-shifted compared to that of the pristine dibenzoazaborine compound (415 nm). Notably, all compounds exhibited near-unity PLQYs, narrow full width at half maximum values (～20 nm), and small Stokes shifts (～11 nm). It has been demonstrated that in conjunction with the π-expansion of the azaborine ring by replacing one phenyl ring with a naphthyl ring, the electron-donating alkyl groups also played a significant role in tuning the bandgap and emission. The details of synthesis and photophysical properties will be discussed along with theoretical studies.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Sterically Shielded Triptycene-Fused Multi-Resonance TADF Emitter for Highly Efficient Deep Blue OLEDs

Hanif Mubarok, Taehwan Lee, Jaehoon Jung, Min Hyung Lee[*]

Department of Chemistry, University of Ulsan, Korea

Multi-resonance (MR) effect-induced thermally activated delayed fluorescence (TADF) based on boron and nitrogen atom is still emanating as a promising material in the area of organic light-emitting diodes (OLEDs). Herein, we report a novel sterically shielded yet extremely rigid emitter, namely Tp-DABNA in which three dimensional triptycene has been successfully fused into the B, N core of MR skeleton. The doped host film of this emitter showed a narrow deep blue emission with a combination of very fast radiative decay rates together with near-unity photoluminescence quantum yield and full width at half maxima (FWHM) of 19 nm. Moreover, when this emitter was co-doped with a TADF sensitizer, the hyperfluorescence (HF) film could significantly suppress the undesirable Dexter energy transfer compared to t-DABNA emitter. The TADF- and HF-OLEDs based on Tp-DABNA displayed highly efficient deep blue emission with improved devices performances and mitigated efficiency roll-offs. Full details of the experimental and computational results will be discussed.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Two silver aminopyridine nitrate complexes with large birefringence

Myung-Ho Choi, Kang Min Ok[1,*]

Division of Chemistry, Sogang University, Korea

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

New silver aminopyridine nitrate complexes, $Ag(C_6H_8N_2)(NO_3)$, and $Ag_2(C_7H_{10}N_2)_2(NO_3)_2$, were obtained using the recrystallization method. Both complexes crystallize in the triclinic space group *P*-1. The $Ag(C_6H_8N_2)(NO_3)$ structure features a one-dimensional framework composed of a linearly coordinated silver cation and a 4-aminomethylpyridine molecule with a nitrate anion. On the other hand, the $Ag_2(C_7H_{10}N_2)_2(NO_3)_2$ structure also consists of a linearly coordinated silver cation with nitrate, but a flexible aliphatic chain of 4-aminoethylpyridine molecules creates a zero-dimensional molecular compound. Both compounds are supported by pyridine-silver-amine bonding with π-π interactions between the two pyridine rings, aligned in an antiparallel manner, and hydrogen bonding between the ligand's amine group and the nitrate anion. The optical bandgaps of the two structures are quite similar: 3.67 eV for $Ag(C_6H_8N_2)(NO_3)$ and 3.73 eV for $Ag_2(C_7H_{10}N_2)_2(NO_3)_2$. However, the calculated birefringence values show a significant difference between them, 0.206 for $Ag(C_6H_8N_2)(NO_3)$ and 0.243 for $Ag_2(C_7H_{10}N_2)_2(NO_3)_2$, respectively. This discrepancy is likely attributed to environmental variations in the π-conjugated system. Detailed characterizations of the reported materials are presented.

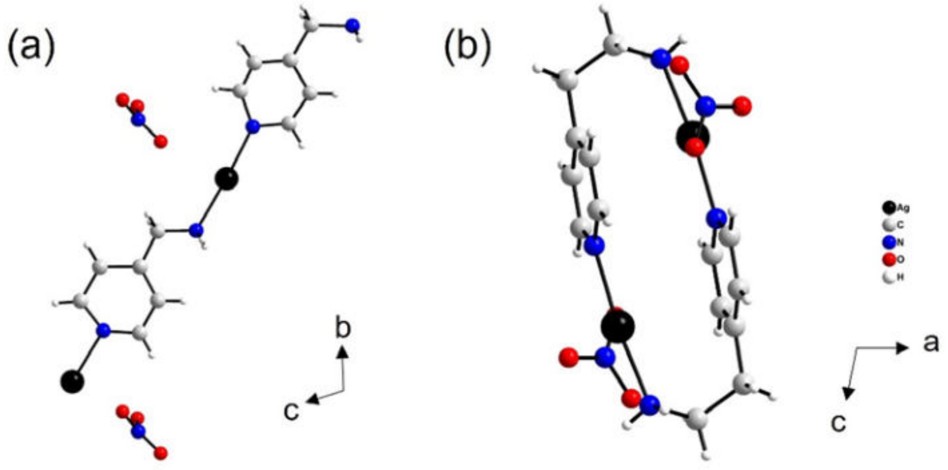


Figure 1. Representation of Ball-and-stick model in the *a*-axis for $Ag(C_6H_8N_2)(NO_3)$ (a), and *b*-axis for $Ag_2(C_7H_{10}N_2)_2(NO_3)_2$ (b) crystallized in *P*-1 (black, Ag; grey, C; red, O; blue, N; and white, H).

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Air-Stable Multi Redox-Active 1,2-Dicarbonyl Radical Cation Stabilized by Naphthoquinone Fused N-Heterocyclic Carbenes

Jaelim Kim, Eunsung Lee*

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

Multi-redox-active organic molecules have been actively investigated for using them as functional materials. Even though organic radicals have excellent redox properties from their unique electronic configuration, there are only a few examples of organic radicals as material because of their synthetic challenge and low stability under various conditions. Herein, we introduced highly stable multi-redox-active 1,2-dicarbonyl radical cation stabilized by naphthoquinone fused N-heterocyclic carbenes (NHCs). This radical cation showed high stability in various conditions such as air, moisture, and heat. Furthermore, it showed three reversible cycles through about the 2 V range in cyclic voltammetry. We successfully synthesized and characterized one-electron-oxidized compound, one- and two-electron-reduced compounds through Density functional theory (DFT), single crystal X-ray diffraction (SCXRD), and electron paramagnetic resonance (EPR). Details will be described in the presentation.

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

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Tetradentate Pt(II) Complexes with a Bulky Substituent for Deep Blue

Hyeok Jin Yu, Rafi Muhammad Lutfi, Min Hyung Lee[1,*]

Chemistry Department, University of Ulsan, Korea

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

Tetradentate Pt(II) complexes have received great interest as efficient blue phosphorescent materials in organic light-emitting diodes (OLEDs) due to their rigid molecular structure and highly phosphorescent nature. However, due to the square planar configuration, Pt(II) complexes may form excimers at high concentrations, which has often led to a reduction in color purity and phosphorescence efficiency. To address this issue, in this study, a sterically bulky substituent, namely triptycenyl (Tp), has been introduced into the imidazole and benzimidazole rings of the ligands. Using the ligands, 4-coordinated Pt(II) complexes (1 and 2) were prepared and characterized. The complexes exhibited deep blue phosphorescence with high quantum efficiency and narrow emission bandwidth. The photophysical properties of 1 and 2 were also compared with the well-known Pt(II) complexes. The details of the synthesis, characterization, and photophysical properties of the complexes will be discussed.

Poster Presentation : **INOR.P-29**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

$Sr(NO_3)(NH_2SO_3)\cdot H_2O$: First Nitrate Sulfamate Revealing Remarkable Second-Harmonic Generation and Enhanced Birefringence with Honeycomb-like Layered Structure

Xuefei Wang, Kang Min Ok[1,*]

Department of Chemistry, Sogang University, China

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

The strategy of synergistically combining mixed chromophores has garnered substantial interest for its ability to leverage the advantages of both groups, leading to innovative nonlinear optical (NLO) materials. We have successfully designed and synthesized $Sr(NO_3)(NH_2SO_3)\cdot H_2O$, a noncentrosymmetric compound, which notably stands as the first reported nitrate sulfamate compound. This compound features zigzag $[SrNO_{10}(H_2O)]_\infty$ infinite layers, forming a honeycomb-like graphene topology in its layered structure. The unique arrangement results in an excellent second harmonic generation (SHG) response, 5.1 times that of KH_2PO_4, and an optimized birefringence of 0.06650 at 532 nm. Furthermore, the presence of interlayered covalent $[NH_2SO_3]$ groups facilitates improved crystal growth behaviors, resulting in a large single crystal with dimensions of $19 \times 17 \times 3.5$ mm^3. This discovery introduces a new class of NLO materials and significantly broadens the horizons of structural chemistry.

Poster Presentation : **INOR.P-30**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Synthesis of Catalysts based on Tridentate Salicylaldimine for the Conversion of Carbon Dioxide into Carbonates

Bokwon Jang

Chemistry, Chungnam National University, Korea

Carbon dioxide is recognized as a primary driver of global climate change and Earth's warming, leading to ongoing research and efforts to both reduce its emissions and explore its utilization. One such area of study involves the synthesis of cyclic carbonates or polycarbonates by reacting epoxides with carbon dioxide, with the aim of commercializing these processes. The role of catalysts in this carbonation process is crucial. We synthesized catalysts necessary for carbon dioxide conversion using zinc and cobalt as central elements, with tridentate salicylaldimine as ligands. In this poster, we will showcase the synthesis process and structure of zinc and cobalt catalysts. Additionally, we will present the results of carbon dioxide conversion experiments conducted under varying reaction conditions, illustrating conversion rates. This will serve to evaluate the efficiency of the catalysts.

Poster Presentation : **INOR.P-31**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Developing zinc(Ⅱ) heterogeneous catalysts for CO_2 conversion to cyclic carbonates.

Hongseo Park

Chungnam National University, Korea

Based on records from the late 19th century to the present, it is evident that as the concentration of carbon dioxide (CO2) in the atmosphere increases, the rate of temperature rise is accelerating. Therefore, a variety of research is being conducted to reduce the CO2 in the atmosphere. One of the carbon capture and utilization (CCU) technologies involves the conversion of CO2 to poly(carbonate) or poly(urethane), which are widely used in various industries [1-3]. In this conversion process, the catalytic system plays a crucial role [2-3]. We have synthesized several zinc complex catalysts with multiple adjacent metal centers for the conversion of CO2 to cyclic carbonates and evaluated their efficiency in catalytic conversion. The synthetic procedures [4-6], analysis, and evaluation of these catalysts will be presented in this poster session.

Poster Presentation : **INOR.P-32**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Chimeric MOFs: SBU Transformation from Zn-cluster to Fe-cluster and Its Effects on Gas Adsorption and Dye Selectivity

Seungwan Han, Seonghwan Lee[1], Myoung Soo Lah[1,*]

PETROCHEMICAL CATALYST RESEARCH CENTER, Korea Research Institute of Chemical Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Symmetry-mismatched SBU transformation is a very rare phenomenon. Connecting the building blocks with a symmetry mismatch is challenging due to the strong strain that disrupts the ordering of the structure. Recently, we introduced a strategic approach to synthesize chimeric MOF with symmetry-mismatched building blocks by utilizing flexible 1,3,5-benzenetribenzoate linker to alleviate framework strain. This approach enables a successful transformation while cleverly maintaining the overall structure of the MOF. Herein, we focus on the shift from a Zn-based MOF containing a [Zn4O(COO)6] secondary building unit (SBU) of octahedral site symmetry (ANT-1(Zn)) to an Fe-based one with a [FeIII3O(COO)6]+ SBU of trigonal prismatic site symmetry (ANT-1(Fe)). This process leads to a reduction in framework volume and pore size, coupled with a shift in the framework’s charge, influencing the MOF's gas and dye adsorption abilities. During the transformation, intermediate core–shell MOFs (ANT-1(Zn@Fe)) are formed, showing unique gas sorption properties and modified preferences for dye adsorption owing to structural changes at the core-shell interface. Heteronuclear clusters located at the framework interfaces enhance the heat of CO2 adsorption and also affect the selectivity for dye size. This research offers valuable insights into fabrication of novel MOFs with unique properties by modifying the SBU of a MOF with flexible organic linkers to transition from one site symmetry to another.

Poster Presentation : **INOR.P-33**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Improved electrooxidation of ammonia via single-atom metal decoration on Platinum Nanocubes.

Juhyun Cho, Jungki Kim[1], Jeonghyeon Kim[2], Saehyun Park[2], Sang-Il Choi[*]

Department of Chemistry, Kyungpook National University, Korea
[1] department of chemistry, Kyungpook National University, Korea
[2] Kyungpook National University, Korea

The global warming crisis is primarily driven by the continuous increase in carbon dioxide emissions. To combat this issue, researchers are exploring various solutions, one of which is the use of ammonia fuel cells or ammonia electrolytic cells. Ammonia is a carbon-free material with a higher energy density and is easier to handle and transport compared to hydrogen. These devices are eco-friendly as they do not produce carbon dioxide as a byproduct, unlike traditional systems that rely on organic matter as a reactant. However, the stability of the anodic reaction ammonia oxidation reaction (AOR) is a significant concern as the catalyst facilitating the reaction is prone to poisoning from N-species intermediates (Nads, NOads). One promising approach to addressing this poisoning phenomenon is the introduction of transition metals into the catalyst. Although the exact cause of the increased resistance to poisoning remains unclear, numerous reports have suggested that stability improves when transition metals such as Ni, Cu, and Ru are added. In our research, we have introduced various transition metals at the atomic level on a platinum nanocube and tested their effectiveness in facilitating the ammonia oxidation reaction.This research has been performed as Project Open Innovation R&D(OTSK_2022_036) and supported by K-water.

Poster Presentation : **INOR.P-34**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Magnesium–Aliphatic Dicarboxylate–Aqua Framework: Glass–Forming Coordination Polymers

Minhyuk Kim, Hoi Ri Moon[1,*]

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

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

Carboxylate-based frameworks are commonly used architectures in metal-organicframeworks(MOFs) or coordination polymers (CPs). However, liquid or glass CPs have been obtained from azole-or weakly coordinating ligand-based frameworks.The strong coordination bonds of carboxylate ligands to metals block the thermal vitrification pathways of MOFs.Were cently announced the first example of a carboxylate-based melt-quenched MOF glass comprising Mg^{2+} and an aliphatic carboxylate ligand, adipate(adp). The low T_m is due to the flexibility and low symmetry of the aliphatic carboxylate ligand(raising entropy of fusion(ΔSfus)) and the lack of crystal field stabilization energy on metal ions(reducing enthalpy of fusion(ΔHfus)).A recent study has demonstrated that coordinated water can weaken the strength of M-L bonding in frameworks, leading to its replacement and consequently accelerating the melting. Building upon this finding and employing our own strategy, we have identified the magnesium-aliphatic dicarboxylate-aqua frameworks (MgC_nDC-aqua, n=2-8) as a promising new family of glass-formable CPs.

Poster Presentation : **INOR.P-35**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Regulation of MMP-2/9 by Natural Products: Implications for Cancer Therapy

Thi Ha Vy Vo, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

For many decades, extensive research efforts have been dedicated to uncovering novel cancer treatments. 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 natural products 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. This study provides novel insights into how flavonoids regulate MMP-2/9. Moreover, it may contribute to the development of another library of natural products for cancer therapy.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-36**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Systematic Investigations of PCN-222 derivatives' Moisture sensitivity prepared for applications of Colorimetric Sensor Arrays.

Dongmin Kim, Jungseok Heo[*]

Department of Chemistry, Chungnam National University, Korea

Colorimetric sensor arrays (CSAs) are immediate and easy analysis method for detecting various volatile organic compounds (VOCs), especially in respiratory diseases. However, since low concentrations of VOCs have low detection limits, experiments should be conducted in an environment where other conditions do not change. Therefore, materials that react well to VOCs but do not react well to other substances should be selected as sensors. Considering the difference in humidity among these, sensors manufactured using PCN-222, porphyrin metal-organic frameworks (MOFs), showed less change when reacted with moisture. Several metals were combined to PCN-222, reacted with moisture, and the amount of color change was compared.

Poster Presentation : **INOR.P-37**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Morphology-Controlled Synthesis of β-FeOOH Nanorods and Their pH-Dependent Formation

Mijin Kim, Hongseok Yun[*]

Department of Chemistry, Hanyang University, Korea

Akaganeite (β-FeOOH) has gained research interest as a potential electrode material for energy storage devices such as Li-ion batteries and supercapacitors due to its natural abundance, high theoretical capacities, low cost, and non-toxicity. In this study, various methods were employed to synthesize β-FeOOH nanorods with controlled particle shapes and aspect ratios. The influence of surfactants on particle morphology was investigated using CTAB, PVA, and SDS. The synthesized β-FeOOH nanorods exhibited distinct shapes depending on the choice of surfactant used. CTAB-assisted synthesis resulted in wide nanorods , while PVA-assisted synthesis yielded relatively thin, elongated, and rough nanorods. By contrast, SDS-assisted synthesis produced triangular particles. We further investigated the pH-dependence of β-FeOOH nanorod morphology, showing decrease of pH promotes the crystallization of β-FeOOH nanorods. Overall, this study demonstrates the successful synthesis of β-FeOOH nanorods with tailored morphologies through the utilization of different surfactants and pH adjustments. These findings contribute to a deeper understanding of the morphological control of β-FeOOH and its potential applications in various fields.

Poster Presentation : **INOR.P-38**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Molecular Geometry Effect for Photoluminescence of 2-Phenylnaphthalene-appended *ortho*-Carboranes

YungJu Seo, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

We synthesized and characterized four 2-phenylnaphthalene appended *o*-carboranyl luminophores, each bearing a different distortional angle of the 2-phenyl ring (1F, 2P, 3M, and 4I). The geometric features around the 2-phenyl ring in the crystalline state were fully determined by single-crystal X-ray diffraction. In both rigid states (solution at 77 K and solid states), all compounds showed intense ICT-based emission in the region of yellowish-green. Interestingly, there was a gradually decreased in the quantum efficiency of the ICT-based emission as the distortion of terminal 2-phenyl ring increased from 1F to 4I. Additionally, the radiative decay constant of 1F was five times higher than that of 4I, while the nonradiative decay of 1F was less than one-third that of 4I. Moreover, theoretical simulation of the low-energy transition in the first excited state of 2P indicated that the degree of distortion in the 2-phenyl ring significantly impacts the efficiency of the ICT-based radiative process. The findings based on theoretical results distinctly demonstrate that the ICT-based radiative efficiency of π–conjugated *o*-carborane is significantly affected by the geometric formation of appended aromatic group.

Poster Presentation : **INOR.P-39**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Modifications of amyloid-β peptides by a mononuclear cobalt complex

Jong-Min Suh, Dongwook Kim[1], Jaeheung Cho[2,*], Kiyoung Park[3,*], Mi Hee Lim[3,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Department of Chemistry, UNIST, Korea*
[3]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

The deposition of amyloid-β (Aβ) aggregates is a major hallmark of Alzheimer's disease (AD), the most common form of dementia. The pathological role of Aβ peptides in AD, however, has not been fully elucidated due to their intrinsically disordered structures and their aggregation-prone nature.[1,2] To advance our understanding of a relationship between Aβ aggregation and toxicity associated with AD, chemical reagents, particularly, transition metal complexes, that can modify Aβ peptides and alter their aggregation profiles, have been developed.[2-5] The limited examples of transition metal complexes that are able to induce modifications of Aβ peptides are known thus far.[3-5] In addition, various modifications cannot be achieved by these metal complexes. In this presentation, we illustrate a mononuclear Co(II) complex capable of carrying out notable modifications onto Aβ peptides, including decarboxylation and deamination, fragmentation, and both, in the presence of O_2. These modifications onto Aβ peptides by the Co(II) complex can redirect their aggregation pathways to yield relatively less toxic aggregates, compared to Aβ aggregates produced without the complex. This work demonstrates that transition metal complexes can be rationally designed to effectively modify amyloidogenic peptides with the consequent impact on their aggregation and toxicity profile.Reference[1] Suh J, Kim M, Yoo J, Han J, Paulina C, Lim MH. Coord. Chem. Rev., 2023, 478, 214978.[2] Savelieff MG, Nam G, Kang J, Lee HJ, Lee M, Lim MH. Chem. Rev., 2019 119, 1221-1322.[3] Suh J, Kim G, Kang G, Lim MH. Inorg. Chem., 2019, 58, 8-17.[4] Kwak J, Woo J, Park S, Lim MH. J. Inorg. Biochem., 2023, 238, 112053.[5] Gomes LMF, Bataglioli JC, Storr T. Coord. Chem. Rev., 2020, 412, 213255.

Poster Presentation : **INOR.P-40**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

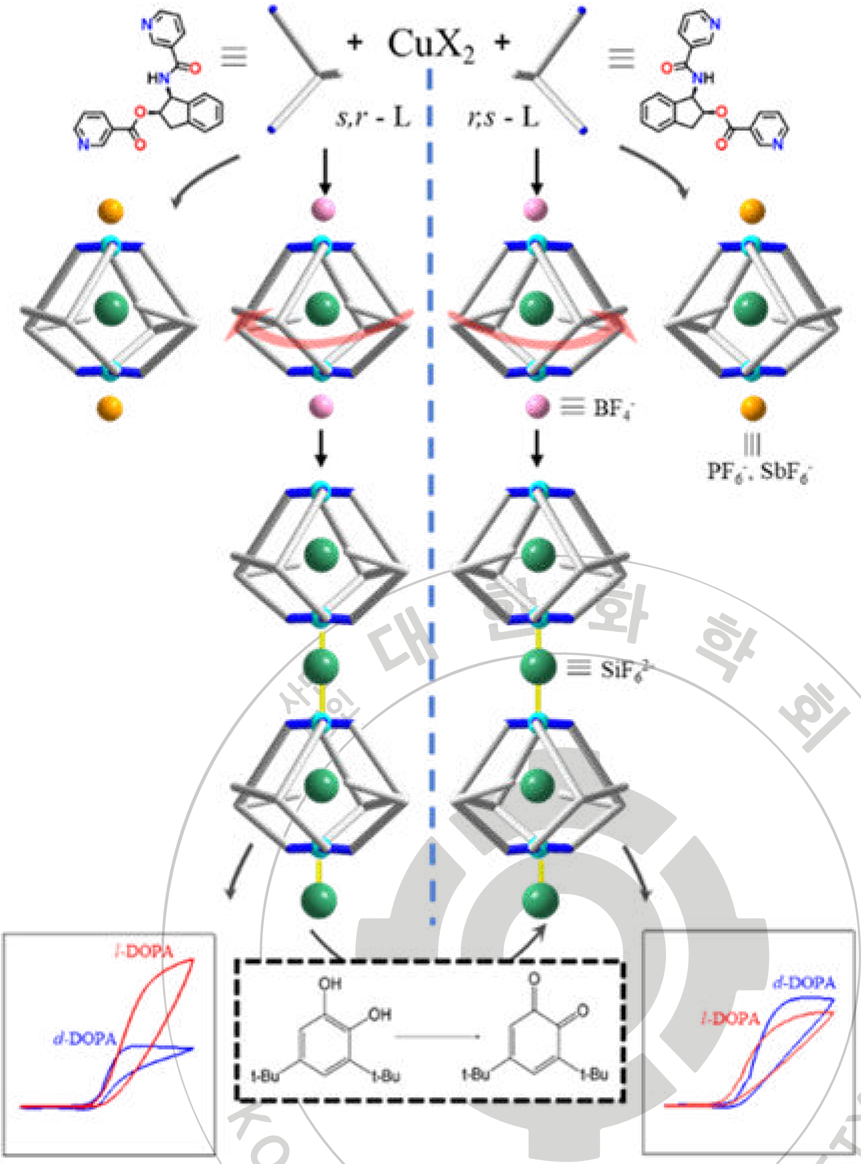
Formation Process of SiF_6@Cu_2L_4 Chiral Cage Pairs in Glass Vessel: Catechol Oxidation Catalysis and Chiral Recognition

Hyo jeong Back, Ok-Sang Jung[1,*]

Pusan National University, Korea

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

Self-assembly of CuX_2($X>^-$= BF_4^-,$PF_6^-$and SbF_6^-) with a pair of chiral bidentate ligands, (1*R*,2*S*)-(+)- and (1*S*,2*R*)-(-)-1-(nicotinamido)-2,3-dihydro-1H-inden-2-yl-nicotinate (*r*,*s*-L and *s*,*r*-L), in a mixture solvent including ethanol in a glass vessel, gives rise to SiF_6^{2-}-encapsulated Cu_2L_4 chiral cage products. The SiF_6^{2-} anion from the reaction of X^- with SiO_2 of the glass-vessel surface acts as a cage template and/or a cage bridge. One of the products, [SiF_6@$Cu_2(SiF_6)$(*s*,*r*-L)$_4$]·$3CHCl_3$·4EtOH, is one of the most effective heterogeneous catalysts for oxidation of 3,5-di-*tert*-butylcatechol. Furthermore, a *l*-DOPA/*d*-DOPA pair is recognizable by the cyclic voltammetry (CV) signals of its combination with chiral cages [SiF_6@$Cu_2(BF_4)_2$(*s*,*r*-and *r*,*s*-L)$_4$]·$4CHCl_3$·2EtOH pair and [SiF_6@$Cu_2(SiF_6)$((*s*,*r*-and *r*,*s*-L)$_4$]·$3CHCl_3$·4EtOH pair.


CuX$_2$
+
+
≡
s,r - L
r,s - L
HN
NH
N
O
≡ BF$_4^-$
≡ PF$_6^-$, SbF$_6^-$
≡ SiF$_6^{2-}$
l-DOPA
d-DOPA
OH
OH
O
O
t-Bu
t-Bu
t-Bu
t-Bu
d-DOPA
l-DOPA

Poster Presentation : **INOR.P-41**

Inorganic Chemistry

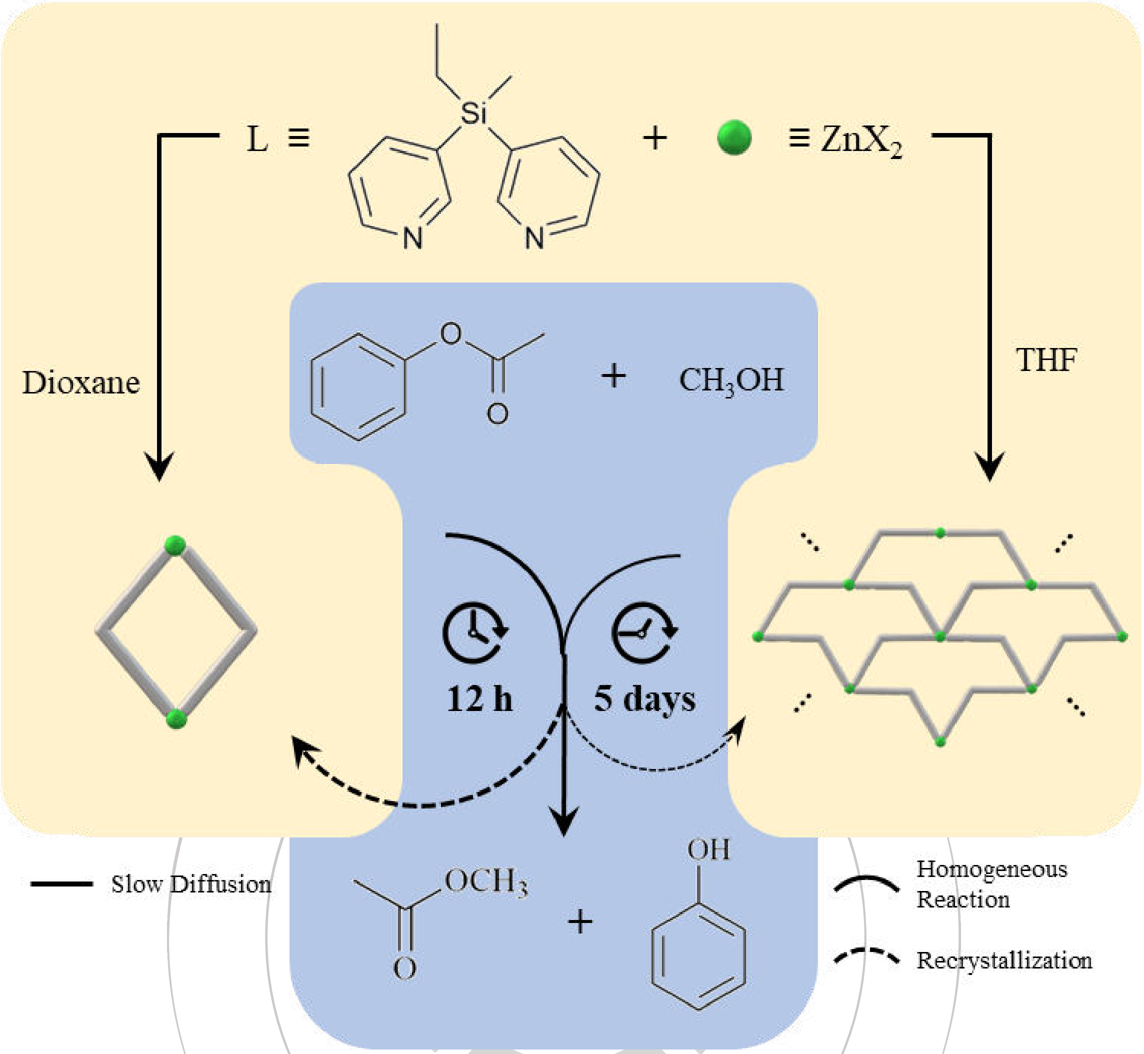
Exhibition Hall C THU 11:00~13:00

High-Yield Recycling of Zn(II) Complexes as Catalysts: Structural Differences via Recrystallization Methods

<u>Jihun Han</u>, 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_3OH
12 h
5 days
OCH_3
O
+
OH
Slow Diffusion
Homogeneous Reaction
Recrystallization

Poster Presentation : **INOR.P-42**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Comparison of Self-Assembled Crystals and Guest-Exchanged Crystals as SCSC Adsorption Matrices in Ni_6L_{12} Ellipsoidal Tubes

Seonghyeon An, Kim Daeun, Ok-Sang Jung[1,*]

Pusan National University, Korea

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

Informative similarities/differences between self-assembled crystals and single-crystal-to-single-crystal (SCSC) guest-exchanged crystals based on both molecular structure and adsorption nature are observed. Self-assembly of $Ni(ClO_4)_2$ with dicyclopentyldi(pyridine-3-yl)silane (L) bidentate in a mixture of toluene and acetonitrile gives rise to purple crystals consisting of double-stranded ellipsoidal tubes, $[Ni_6(ClO_4)_4 (CH_3CN)_8L_{12}]8ClO_4{\cdot}4CH_3CN{\cdot}5C_7H_8$. The coordinated acetonitriles as well as the solvates are removed at 170°C to transform the purple crystals into blue crystals of $[Ni(ClO_4)_2L_2]_n$ that return to the original crystals in the mixture of toluene and acetonitrile. Further, the toluene and acetonitrile solvates of the original crystals are replaced by *o*-, *m*-, and *p*-xylene isomers within 5 min in an SCSC manner. In the present study, SCSC xylene-exchanged crystals were compared with crystals obtained from direct self-assembly in the mixture of each xylene isomer and acetonitrile.

Poster Presentation : **INOR.P-43**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Dimensional Transformation of Cage Compounds: Conversion into 3D Networks through a Simple Method

Gyeongmin Kim, Ok-Sang Jung[1,*]

Department of chemistry, Pusan National University, Korea

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

Dimensional transformation of a cage compound into 3D networks through a simple method. The self-assembly of zinc nitrate hexahydrate ($Zn(NO_3)_2,6H_2O$) and a new ligand, tris(2-(isoquinolin-5-yloxy)ethyl)amine (L), in dioxane and acetonitrile resulted in the formation of single crystals composed of the M_3L_2 cage. In benzene and ethanol resulted in the formation of single crystals composed of the 3D networks. When the single crystal of M_3L_2 is immersed in ethanol, a condition for forming a 3D structure, it is recrystallized into a 3D structure.

Poster Presentation : **INOR.P-44**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

[Withdrawal] Facile Fabrication of Homochiral MOF Composite Membrane for Efficient Chiral Separation via Templated Strategy

Dongjun Shin, Jin Yeong Kim[1,*]

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

Poster Presentation : **INOR.P-45**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Construction of Photoreactive Zinc(II) Metal-Organic Frameworks with *cis*- and *trans*-Stereoisomers

Jaewook An, Jihye Oh, In-Hyeok Park[*]

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

We report the synthesis of two metal-organic frameworks (MOFs) with different structures under the same solvothermal reaction conditions, depending on the *cis*- or *trans*- stereo isomers of the ligands. Furthermore, the single-crystal to single-crystal (SCSC) transformation of these MOFs are structurally characterized. These two types of MOFs were synthesized by the self-assembly reaction of $Zn(NO_3)_2{\cdot}6H_2O$, 4-styrylpyridine (spy), and two forms of cyclohexane dicarboxylic acids (*cis*-chdc and *trans*-chdc). This resulted in the synthesis of $[Zn_2(spy)_2($*cis*-chdc$)_2]$ (**1**) and $[Zn(spy)_2($*trans*-chcd$)]$·spy (**2**). MOF **1** features Zn(II) dinuclear repeating units and adopts a 1D structure. The coordination environment of Zn(II) involves five-fold coordination within a square pyramid coordination environment. In contrast, MOF **2** exhibits Zn(II) mononuclear repeating units and a 1D structure, with a four-fold coordination environment within a tetrahedral coordination environment. Notably, spy molecules are guests between the frameworks in MOF **2**. Both MOFs **1** and **2** exhibit complete photoreactivity with a yield of 100%. The coordinated spy in both MOFs align head-to-tail with those in adjacent frameworks, satisfying Schmidt's criteria for their distance.[1] Upon undergoing a photoreaction, the structure of MOF **1** changes to $[Zn_2($*rctt*-ppcb$)($*cis*-chdc$)_2]$ (**3**), leading to a shift from 1D to 2D dimensionality, where *rctt* = *regio, cis, trans, trans*; ppcb = 1,3-bis(4'-pyridyl)-2,4-bis(phenyl)cyclobutane. In the case of MOF **2**, upon undergoing a photoreaction, the structure of MOF **2** transforms to $[Zn($*rctt*-ppcb$)($*trans*-chdc$)]$·spy (**4**), which was confirmed by ^{1}H nuclear magnetic resonance (NMR) and powder X-ray diffraction (PXRD) analyses. Further details will be discussed in the poster section.

Reference

[1] G. M. J. Schmidt, Photodimerization in the solid state, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-46**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Structural and Photoreactivity Differences in Zn(II) Metal-Organic Frameworks with Stereoisomers

Jihye Oh, Jaewook An, In-Hyeok Park[*]

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

In this study, Zn(II) based metal-organic frameworks (MOFs) were synthesized using two types of cyclohexanedicarboxylic acid (chdc) stereoisomers, resulting in distinct MOF structures containing *cis*- and *trans*-chdc, respectively. MOF **1** and **2** were synthesized under the same solvent conditions using Zn(II) salt, 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb), and the chdc ligands through a solvothermal reaction. In the case of the $[Zn_2(bpeb)(\textit{cis}\text{-}chdc)_2]\cdot xDMA$ (**1**) containing *cis*-chdc, it exhibited a single-pillared two-dimensional (2D) layer structure. On the other hand, for the $[Zn(bpeb)(\textit{trans}\text{-}chdc)]\cdot xDMA$ (**2**) containing *trans*-chdc, it displayed a double-pillared 3D structure in a 2-fold interpenetration. Due to the structural differences arising from the use of different chdc isomers, they exhibit distinct [2+2] cycloaddition reaction tendencies. MOF **1**, with its single-pillared structure, exhibited larger distances between double bonds of bpeb, [2+2] cycloaddition reaction cannot take place. The double-pillared structure of MOF **2**, in which the distance between the double bonds of bpeb was close, satisfied the conditions for photochemical reactions to proceed. Consequently, the formation of in-phase single photoreaction products was confirmed by ^1H NMR analysis.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-47**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Emissive Supramolecular gel of 1-Pt(II) Complexes

Hyoungwook Kang, Eungyu Lee, Jong Hwa Jung[1,*], Sung Ho Jung[2,*]

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

Utilizing metal-ligand binding plays an important role in regulating the photophysical properties of supramolecular gels. In this study, we designed 1-Pt complexes, composed of a benzene- 1,3,5-tricarboxamide (BIA) central unit functionalized with three terpyridines, which can form supramolecular gels with Pt(Il) in DMSO/water mixtures. The resulting supramolecular gel 1-Pt, exhibited strong orange emission, originating from the metal-to-metal ligand charge transfer (MMLCT) in gel formation. Furthermore, the temperature-dependent absorption spectra changes of the supramolecular polymer 1-Pt showed a non-sigmoidal transition, following a cooperative pathway involving a nucleation-elongation mechanism.

Poster Presentation : **INOR.P-48**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

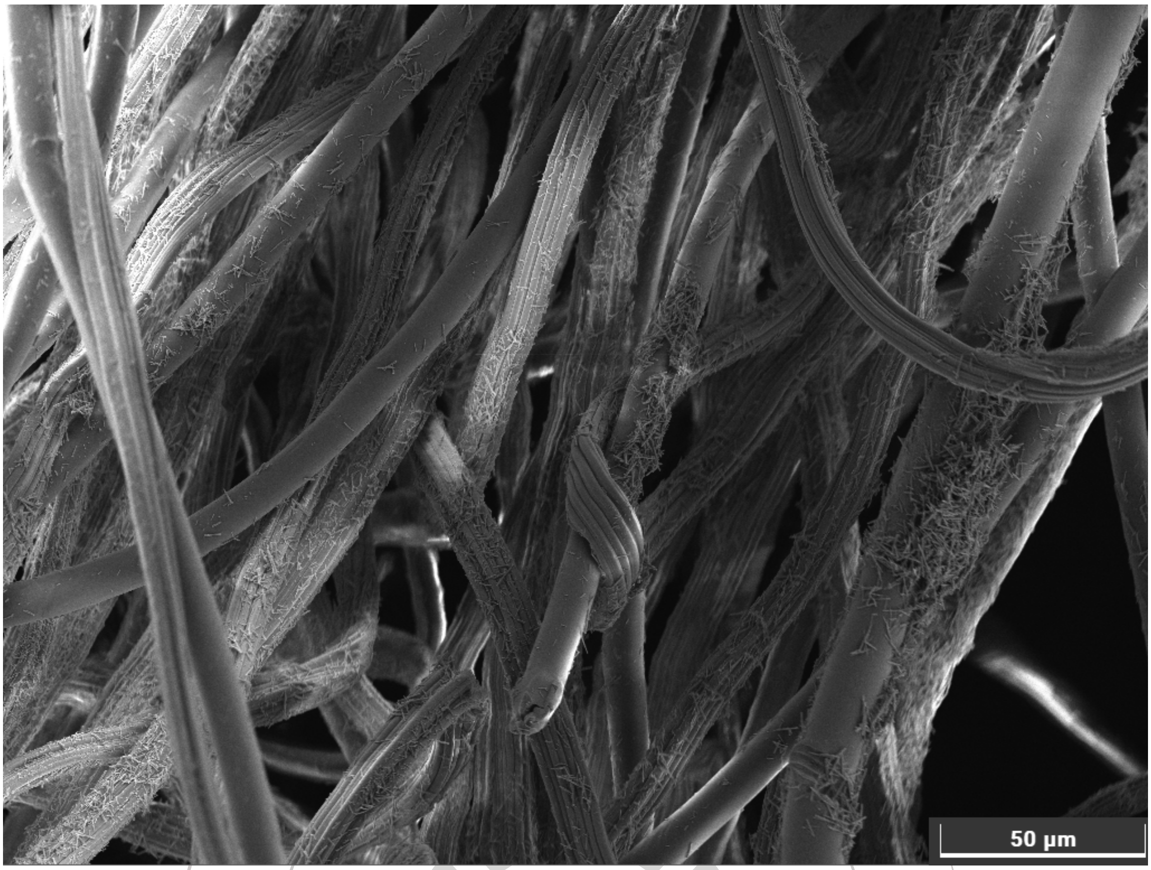
Sensitivity Optimization of Colorimetric Sensor Array in terms of concentrations of MOFs particles

Seung Yun Oh, Jungseok Heo[1,*]

chemistry, Chungnam National University, Korea

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

Based on a previous study, this research was conducted to investigate the tendency of sensor detection behaviors at various concentrations of MOF. Colorimetric sensing, a rapid and straightforward method for analyzing diverse chemicals, was employed. Porphyrin derivatives have proven to be excellent chromogenic materials for VOC detection. In order to maximize gas sensing capabilities, we introduced porphyrin MOF derivatives with microporous structures and examined their gas sensing properties for VOCs. However, the porphyrin structure's drawback is its costliness. Therefore, our aim is to assess changes in efficiency based on concentration to determine optimal conditions. The results will be presented through a poster, utilizing color difference maps and graphs.


50 μm

Poster Presentation : **INOR.P-49**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and structural and electrochemical properties of 1,1-Disubstituted-benzosiloles

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. 1,1-Disubstituted-benzosiloles (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 1,1-diphenylbenzosilole 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).

Poster Presentation : **INOR.P-50**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Structural, Spectroscopic Characterization and Reactivity of Manganese(III)-Peroxo Intermediate: Deformylation Reaction of 2-PPA via Initial *α*-H Abstraction

Akhilesh Kumar, Yong-Min Lee[1], Wonwoo Nam[2,*]

Chemistry & Nanobio Energy Materials Center, EWHA WOMANS UNIVERSITY, India

[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*

[2]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

Metal-peroxo intermediates play a pivotal role in the catalytic mechanism of nonheme metalloenzymes. However, the precise understanding of their chemical properties and reactivity study remain elusive. In this study, a mononuclear nonheme manganese(III)-peroxo intermediate, $[Mn^{III}(O_2)(12\text{-TBC})]^+$ (**1**), was generated by reacting $[Mn^{II}(12\text{-TBC})]^{2+}$ and H2O2 in the presence of Et_3N at 20 °C and characterized by various spectroscopic techniques, such as X-ray, ESI-MS, and EPR spectroscopies. A parallel mode spectrum of **1** purified sample of the bluish-green intermediate shows a characteristics Mn(III) feature at $g = 8.3$. Because of the high thermal stability of the intermediate **1**, we were able to obtain single crystals suitable for XRD experiments. The crystal data suggests that Mn(III) complexes bound with O_2 unit with side-on fashion and the O-O bond distance is 1.36 Å, typically for the peroxo bound to transition-metal ion. Subsequently, we investigated the deformylation behavior of compound **1** in a reaction with 2-phenylpropionaldehyde (2-PPA). To understand the details of the rate-determining step for the reaction of **1**, we decided to investigate the kinetic isotope effect (KIE) for replacing the α-hydrogen atom with deuterium. Upon addition of *α*-[D1]-PPA (~ 94 %, D-enriched) to **1** which shows the KIE = 2.1, and it can be concluded that the reaction has a rate-determining hydrogen atom abstraction step.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-51**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

A Nonheme Iron(III)-Peroxo Intermediate as a Functional Model of Rieske Dioxygenases

Wenjuan Zhu, Yong-Min Lee[1], Wonwoo Nam[2,*]

Department of Chemistry and Nanoscience, Ewha Womans University, China
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

The nature of the reactive intermediates and the mechanism of the cis-dihydroxylation of arene and olefin double bonds by Rieske dioxygenases have been the topic of intense research over the several decades. In this study, a mononuclear nonheme iron(III)-peroxo complex bearing *N*-tetramethylated 12-membered cyclam, $[\mathrm{Fe^{III}(O_2)(12\text{-}TMC)}]^+$, was synthesized and characterized spectroscopically; the characterization with EPR, Mössbauer, XAS, and rRaman spectroscopies supported a high-spin S = 5/2 Fe(III) species binding a side-on O_2-unit in $[\mathrm{Fe^{III}(O_2)(12\text{-}TMC)}]^+$ complex. A notable observation was that $[\mathrm{Fe^{III}(O_2)(12\text{-}TMC)}]^+$ was demonstrated to be reactive towards olefins and α-substituted naphthalene, producing $\mathrm{Fe^{III}}$-cycloadducts (e.g., $[\mathrm{(12\text{-}TMC)Fe^{III}}$(1-phenylethane-1,2-bis(olate))$]^+$ and $[\mathrm{(12\text{-}TMC)Fe^{III}}$(cyclooctane-1,2-bis(olate))$]^+$); these products were successfully isolated and analyzed by various structural and spectroscopic methods. Upon the addition of acid, these $\mathrm{Fe^{III}}$-cycloadducts undergo a transformation leading to the formation of the corresponding *cis*-diol products. The current investigation provides the first conclusive experimental evidence demonstrating that a synthetic $[\mathrm{Fe^{III}(O_2)(12\text{-}TMC)}]^+$ complex serves as the active intermediate responsible for the *cis*-dihydroxylation of olefins and arenes by Rieske dioxygenases and bioinspired nonheme iron catalysts. Moreover, the present results support the structure of NDO binding dioxygen in a side-on fashion as the reactive species for the NDO-mediated *cis*-dihydroxylation of naphthalene.

Poster Presentation : **INOR.P-52**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Nonlinear Acid Promotion in Oxidation of Substrates by Mononuclear Nonheme Iron(III)-Aqua Complexes

Madhuri Nilajakar, Yong-Min Lee[1], Shunichi Fukuzumi[2,*], Wonwoo Nam[3,*]

Department of Chemistry and Nanoscience, Ewha Womans University, India
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Department of Chemistry, University of Tsukuba, Japan*
[3]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

Binding of more than one acid molecule to metal-oxygen intermediates is expected to enhance the oxidation reactivity, exhibiting a higher order dependence of the rate constant on the acid concentration than the first-order. Such nonlinear dynamics of electron transfer (ET) may open a new frontier of ET chemistry as nature has already developed in contrast to the artificial systems. In the present study, we report that binding of not only one but also two triflic acid (HOTf) molecules to mononuclear nonheme iron(III)-aqua complexes, $[(dpaq)Fe^{III}(OH_2)]^{2+}$ {**1**: dpaq = 2-[bis(pyridin-2-ylmethyl)]amino-*N*-(quinolin-8-yl)acetamidate} and $[(tdpaq)\ Fe^{III}(OH_2)]^{2+}$ {**2**: tdpaq = 2-[benzyl(pyridin-2-ylmethyl)amino] -*N*-(quinolin-8-yl)acetamidate}, results in enhancement of the oxidation reactivity of the iron(III)-aqua complexes to exhibit the first and second-order dependence of the rate constant on concentration of HOTf. The rate constants of ET and oxygen atom transfer (OAT) of **1** and **2** exhibit the second-order dependence on [HOTf], whereas those of hydrogen atom transfer (HAT) of **1** and **2** exhibit both the first-order and second-order dependence on [HOTf], accompanied by the change in the deuterium kinetic isotope effects. The dependence of logarithm of the rate constants of acid-promoted oxidation reactions by **1** and **2** on the ET driving force was well evaluated in light of the Marcus theory of outer-sphere ET to discuss the acid-promoted oxidation mechanisms by **1** and **2**. This is the first time to report nonlinear acid promotion in oxidation of substrates by metal-aqua complexes.

Poster Presentation : **INOR.P-53**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Regulation of C-H and O_2 activation through auxiliary components

Yunha Hwang, Gayeon Shin, Yerim Park, Seung Jae Lee[*]

Department of Chemistry and Institute of Molecular Biology and Genetics, Jeonbuk National University, Korea

Hydroxylation of soluble methane monooxygenase (sMMO) has been studied extensively to understand biological conversion from methane to methanol in ambient conditions, although more detailed mechanisms of this biocatalyst still needs to be investigated. The structures of hydroxylase (MMOH), MMOB and two MMOR domains have been determined through X-ray crystallography and nuclear magnetic resonance (NMR) studies. Potential roles in the catalytic reaction have been proposed based on these structural and spectroscopic studies. Unfortunately, structures of MMOH complexed with other enzymes have made it difficult to fully elucidate the molecular mechanisms by which MMOH through the dynamic association with its auxiliary components. In this presentation, structural and functional aspects of sMMO components including hydroxylase (MMOH), regulatory component (MMOB) component and inhibitory enzyme (MMOD) will be discussed through the complex structures. The other auxiliary enzyme MMOR transfers electrons from NADH to diiron active sites through FAD-binding domain and ferredoxin domain. This electron transfer mechanism can be explained by electron paramagnetic resonance (EPR) studies by annealing methods to extract $[2Fe\text{-}2S]^+$ and FAD and domain species at 20 and 60 K, respectively. The advanced techniques from ENDOR and ESEEM confirmed that neutral flavin is a major reduced form and Cys50 coordinated iron is easily oxidized to Fe^{3+}.

References

1. Lee, C. Hwang, Y., Kang, H, G. Lee, S. J., “Electron transfer to hydroxylase through component interactions in soluble methane monooxygenases”, *J. Microbiol. Biotechnol.*, 2022, *32*, 287-293.
2. Han Sol Jeong, et al., “EPR-derived Structures of Flavin Radical and Iron-Sulfur Clusters from *Methylosinus sporium* 5 Reductase”, *Inorganic Chemistry Frontiers*, 2021, *8*, 1279–1289.

3. Hanseong Kim, et al., “MMOD-induced Structural Changes of Hydroxylase in Soluble Methane Monooxygenase”, *Science Advances*, 2019, *5*, eaax0059.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-54**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Selective Anaerobic Photocatalytic Oxidation of 5-Hydroxymethylfurfural to 2,5-Diformylfuran by Gold-Exchanged CdS cluster in Zeolite Y Framework

Jeong Eun Kim, Hyun Sung Kim[1,*]

department of chemistry, Pukyong National University, Korea

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

Producing high-value-added chemicals from biomass constitutes a vital research pursuit, offering a pathway to enhance sustainability. Among these prospects, the conversion of 5-Hydroxymethylfurfural (HMF) into a valuable intermediary, such as 2,5-Diformylfuran (DFF), via redox reactions holds prominence. In our preceding endeavors, we substantiated the applicability of gold and CdS-based heterogeneous photocatalysts as fitting semiconductor materials for selectively oxidizing HMF. Additionally, we successfully synthesized Au_2S@CdS clusters within a zeolite framework, establishing a photocatalyst primed for the highly selective oxidation of HMF under anaerobic conditions. Remarkably, the optimal photocatalyst material emerged as a high silica zeolite (Si/Al=30). Enhanced photocatalytic efficiency was realized through the amplification of CdS clusters within zeolite Y, achieved through repetitive CdS synthesis. Moreover, our investigations unveiled that the incorporation of Au_2S, facilitated by gold ion exchange, augments the photocatalytic activity of CdS/zeolite Y, leading to a commendable DFF yield (~46%) over a 4-hour irradiation period. This study effectively demonstrates the synergistic interplay between the heterogeneous photocatalytic attributes of Au_2S@CdS and the supportive impact of zeolite Y. Furthermore, it introduces a novel perspective on the CdS/zeolite composite system, positioning it as a proficient photocatalyst for HMF oxidation reactions.

Poster Presentation : **INOR.P-55**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Substitution of xenobiotic metal ions for the structural zinc finger domains

Yunha Hwang, Hanbin Son, Ka Young Son, 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 coordinates to cobalt in the E. coli system. Iron and copper cannot replace metal ions in PARIS, although iron improves the expression level of zinc-bound proteins. In addition, proteins was expressed and purified for basic characterization and showed cobalt-binding abilities.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-56**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

High-Performance Lithium Metal Batteries Using Wrinkled-Multilayered Graphene

Sangyeop Kim, Na Yeong Kim[1], 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 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, wrinkled-multilayered graphene (WMG) is used as a host for the lithium metal batteries. WMG exhibits lithiophilic surface and mechanical flexibility and robustness, resulting in reduction of dendrite formation and tolerance to the volume change. As a result, WMG-based lithium metal batteries showed outstanding rate performance and long-term stability essential for implementing advanced electrochemical storage systems.

Poster Presentation : **INOR.P-57**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

De novo Design of Dinuclear Metal Complexes for Discriminating between Normal Cell and Colorectal Cancer Cells

Yougang Kim, Hyungbin Park, Chaewon Ahn[1], Yerin Lee, Seungwoo Hong[*]

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

[1]Department of Chemistry, Sookmyung Women's University, Korea

As of now, heavy metal-based drugs are used as anticancer agents, but their non-negligible cytotoxicity and significant side effects necessitate discovering novel compounds capable of selectively targeting cancer cells. Specifically, only the iron complex among first-row transition metal complexes induced apoptosis in colorectal cancer cells. Other metal complexes exhibited minimal anti-proliferative activity. Building upon this, the ligand in the mononuclear complex was modified to synthesize dinuclear biomimetic compounds. Biomimetic metal complexes containing two picolylamine linked by bridging ligand, [M(Bn(N3O2)2)]2+ (M = Mn, Fe, Co, Cu; Bn(N3O2)2 = bridging ligand with picolylamine linked by 2,2'-(1,3-phenylenebis(methylene))bis(oxy)bis(ethane-2,1-diyl)), were synthesized and characterized using various spectroscopic methods, including X-ray crystallography. Their dioxygen and ROS activation reactivity were evaluated both in situ and in vitro. To explore potential synergistic effects compared to the previously reported mononuclear complexes, the cytotoxicities of freshly synthesized dinuclear complexes were conducted to various cancer cells, including colorectal cancer, breast cancer, liver cancer, and renal cancer, but no cytotoxicity was observed in normal skin cell. This indicate that dinuclear complexes show cancer-specific antitumor activity. Among these complexes, the copper complex Cu2(Bn(N3O2)2)(Cl)4 showed significant anticancer activity on liver and renal cancers. Cell viability studies were performed on colorectal, breast, liver, and renal cancer cells, revealing positive effects, particularly in liver and renal cancers. This could be attributed to the arrangement of two N3O2 ligands facing each other, enhancing dioxygen or ROS reaction reactivity.

Poster Presentation : **INOR.P-58**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Unlocking the Potential of Copper Complex in Triple-Negative Breast Cancer: A Superoxide Dismutase Mimicking Model

Chaewon Ahn, Hyungbin Park[1], Yougang Kim[1], Yerin Lee[1], Hangil Lee[*], Seungwoo Hong[1,*]

Department of Chemistry, Sookmyung Women's University, Korea

[1]*Department of Chemistry & Nanoscience, Ewha Womans University, Korea*

One significant development in current cancer chemotherapy is the development of metal complexes with platinum central atoms, such as cisplatin, carboplatin, and oxaliplatin. However, the range of cancers that can be treated with platinum agents is narrow, and the drugs are associated with several side effects and problems of resistance phenomena.In response to these challenges, numerous research groups have endeavored to replace heavy metal-based drugs with less toxic first-row transition metal-based therapeutics, owing to their versatile electronic and structural features. Among the first-row transition metal complexes, copper complexes are promising as anticancer agents because of their anticancer activity through disrupting various cellular processes.Previous research has shown that the $[Cu(bsc\text{-}Bn)]^{2+}$ complex catalyzes the disproportionation of intracellular reactive oxygen species, such as superoxide anion, into hydrogen peroxide and molecular oxygen. Therefore, the decrease in intracellular ROS levels resulted in inhibition of ATP formation, the occurrence of cell cycle arrest, and the induction of apoptosis in colorectal cancer cells.In this study, we have undertaken a novel approach to treat the MDA-MB-468, triple-negative breast cancer (TNBC) cell line, using the Cu complex. As in colorectal cancer cells, the Cu complex was effective against MDA-MB-468 even at low concentrations. It was found that $[Cu(bsc\text{-}Bn)]^{2+}$ complex that mimics superoxide dismutase (SOD) disrupts intracellular redox balance and induces apoptotic signaling pathway. This study proposes the potential to treat triple-negative breast cancer, which is a more aggressive type of tumor with a faster growth rate.

Poster Presentation : **INOR.P-59**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Heterojunction of TiO_2 and methylammonium (MA) lead halide for enhancing photocatalytic HMF oxidation

Yujin Jeong, Hyun Sung Kim*

Department of Chemistry, Pukyong National University, Korea

Perovskite nanocrystals (PNCs) exhibit remarkable catalytic efficiency in the selective oxidation of biomass-derived 5-hydroxymethylfurfural (HMF) to yield 2,5-diformylfuran (DFF). PNCs, extensively investigated for their applications in solar cells and photovoltaics, possess optical and electronic characteristics encompassing high photoluminescence (PL) attributes, adjustable band gaps, and a narrow emission bandwidth. However, structural fragility is observed in PNCs when subjected to diverse environmental conditions like moisture, heat, and light. Diverging from previous methodologies where perovskite was encapsulated with TiO_2, our study introduces a distinctive approach. Herein, methylammonium (MA) lead halide perovskite ($MAPbX_3$, X = Cl, Br, and I) is cultivated through perovskite passivation on TiO_2, resulting in the configuration $MAPbX_3@TiO_2$. This scheme leverages TiO_2's propensity to foster charge transfer by establishing a heterojunction with the perovskite. Furthermore, TiO_2 underwent methylation post APTMS treatment to enhance charge transfer efficiency alongside the perovskite. The study thereby introduces a novel strategy for constructing perovskite-based heterojunctions.

Poster Presentation : **INOR.P-60**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Investigation for Enhancing the Stability of Lead Halide Perovskite QDs During Photooxidation of 5-Hydroxymethylfurfural

Jaemin Han, Hyun Sung Kim*

Department of Chemistry, Pukyong National University, Korea

Nowadays, lead halide perovskite quantum dots (QDs), have garnered significant attention for their potential usage as photocatalysts. In this work, we employ $MAPbX_3$ perovskite QDs as a photocatalyst for the selective oxidation of 5-Hydroxymethylfurfural (HMF) to 2,5-Diformylfuran (DFF) using visible light under aerobic conditions. We synthesized various halide compositions of the catalyst following the LARP method. When we employed with a wide band gap catalyst with a relatively low VBM like $MAPbBr_2Cl_1$~Br_1Cl_2 led to complete oxidation of HMF within approximately 1.5 hours, yielding around 65% with a selectivity of about 97%. A minor product, 5-Formyl-2-furancarboxylic acid (FFCA), was also obtained with a selectivity of around 3%. Nonetheless, similar to some other studies utilizing lead halide perovskites as photocatalysts, the photoluminescence (PL) intensity and photocatalytic efficiency significantly decreased after 3 cycles of photoreaction. To address this issue, we investigated the solvent effect. Initially, we created a mixed solvent system combining ethyl acetate (EtOAc) and a non-polar solvent, but no positive impact on catalytic efficiency and yield was observed. Subsequently, we explored various acetate solvents such as methyl acetate (MeOAc), propyl acetate (PrOAc), and butyl acetate (BuOAc). In the initial reaction, BuOAc exhibited a higher yield of DFF compared to EtOAc, but over a series of reactions, it demonstrated less catalyst durability than EtOAc. Lastly, we managed to regenerate the catalyst by introducing octylamine as an additive in each purification procedure between cycles. With this treatment, we were able to maintain catalytic activity over 6 reaction cycles, as well as the PL intensity.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-61**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Selective Oxidation of a Mustard Gas Simulant by Tris(2,2´-bipyridine)ruthenium(II) Encapsulated in Zeolite Y with Varied Si/Al Ratios

Sumin Kim, Hyun Sung Kim[*]

Department of Chemistry, Pukyong National University, Korea

Sulfur mustard gas, commonly known as HD, stands as one of the primary chemical warfare agents, causing the loss of thousands of lives and extensive contamination. Swiftly developing functional materials to detoxify sulfur mustard within minutes is of paramount importance in safeguarding the lives of those affected. This study centers on heterostructure photocatalysts, constructed by encapsulating varying quantities of tris(2,2´-bipyridine)ruthenium(II) ($Ru(bpy)_3^{2+}$) into zeolite Y (Si/Al ratios: 2.8, 5.0, 12, 30, 60) through the ship-in-a-bottle technique. When exposed to visible light, the photocatalyst generates singlet oxygen ($^1O_2$) which selectively oxidizes a sulfur mustard simulant, 2-chloroethyl ethyl sulfide (CEES), into the non-toxic byproduct 2-chloroethyl ethyl sulfoxide (CEESO). The photocatalyst composed of zeolite Y with a Si/Al ratio of 30 exhibited the highest photocatalytic efficiency, completely converting CEES to CEESO within less than 15 minutes under aerobic conditions. This presentation sheds light on the influence of varying Si/Al ratios of zeolite Y, elucidating distinct photocatalytic activities in detoxifying this perilous chemical warfare agent.

Poster Presentation : **INOR.P-62**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Transition metal complexes and main group phosphorus compounds of a tetradentate ligand with a urea backbone

Dabeen Hong, **ChanHo Jeong**[1], **Kyounghoon Lee**[2,*]

Department of Chemistry Education, Gyeongsang National University, Korea
[1]*Chemisty education, Gyeongsang National University, Korea*
[2]*Department of Chemical Education and Research Institute of Natural Sciences, Gyeongsang National University, Korea*

Transition metal complexes with tetradentate [NNNN] ligands have been used for stoichiometric and catalytic reactions due to their robustness and strong donating abilities. A ligand with a urea-backbone has been underexplored although the urea backbone containing an acute bite angle could manipulate the electronic structure of transition metal complexes. Here we report the ligand design, transition metal complexes, and main group phosphorus compounds of a tetradentate [NNNN] ligand (1). Treatment of 1 with $NiCl_2$(DME) (DME = dimethoxyethane) in the presence of two equivalents of NaOtBu formed a binuclear Ni(II) complex (2), presumably due to the acute bite angle of urea backbone. Similarly, a binuclear Cu(I) complex (3) was prepared by the treatment of 1 with two equivalents of CuCl and NaOtBu. In addition, treatment of 1 with PCl_3 or Cl_2PPh in the presence of NEt_3 formed phosphorus compounds (4 and 5) with distorted geometry around the phosphorus atoms as shown in the crystal structures. The applications of transition metal complexes and main group phosphorus compounds are underway.

Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Fluorescence Properties of Dicationic Pyrene-Based Chromophores Encapsulated in In-MOFs

Jongseo Kim, Seong Huh*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

The emission properties of chromophores are very sensitive to their environments. Different solvents often significantly alter the emission properties of chromophores. Recently, we are investigating the photophysical properties of cationic chromophores captured inside the channels of metal-organic frameworks (MOFs). Simple encapsulation of cationic guest ions into pre-organized MOF channels can be an effective method for controlling the emission properties of chromophores. In this study, two similar dicationic pyrene-based chromophores, $[\text{pyrene-Me}]^{2+}$ and $[\text{pyrene-Et}]^{2+}$ were successfully encapsulated into two isostructural anionic frameworks of InBTB and InTATB, where BTB^{3-} = 1,3,5-benzenetribenzoate and $TATB^{3-}$ = 4,4',4''-s-triazine-2,4,6-triyltribenzoate. We investigated the encapsulation of the dicationic chromophores using UV/Vis-absorption spectroscopy. The fluorescence properties of pyrene-Me@InBTB, pyrene-Me@InTATB, pyrene-Et@InBTB, and pyrene-Et@InTATB were systematically investigated using steady-state fluorescence measurements in solid state. The different fluorescence properties will be discussed.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-64**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Size-tunable mesoporous carbon spheres for high-performance supercapacitors

InCheol Heo, Yejun Ham[1], Won Cheol Yoo[2,*]

Department of Applied chemistry, Hanyang University, Korea
[1]Department of Chemical and Molecular Engineering, Hanyang University, Korea
[2]Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea

Due to their exceptional properties such as lightweight, high electrical conductivity, specific surface area (SSA), adjustable pore structures, and desired surface characteristics, carbonaceous materials have substantial interest as electrode materials for supercapacitors (SCs). In attempts to achieve high energy density, ionic liquid (IL) electrolyte is has attracted great attention Because it can be used in a wide voltage range. However, initial attempts to incorporate IL into SCs encountered challenges, as the large and sluggish ions struggled to effectively access the narrow pores of conventional microporous carbons. In addressing this issues, we have synthesized mesoporous carbon spheres (MCSs) that were produced via co-assembly of polymer and silica sphere (20-50 nm). The interconnected large mesopores facilitated ion mass-transport and thereby efficient utilization of the carbon electrode's surface for capacitive energy storage. The MCS-based SCs demonstrated a high capacitance (328.93 F g^{-1}) and ultrahigh energy density (182.7 Wh kg^{-1}), comparable to the best results reported to date.

Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

CO2 Hydrogenation Catalyzed by an rigidified (PNP)Ru(II) Scaffold

Juwon Paik, Yunho Lee[*]

Department of Chemistry, Seoul National University, Korea

Upcycling technology of CO2 to methanol by transition metal catalytic reactions is receiving much attention. Homogeneous catalytic systems based on organometallic complexes supported by pincer-type ligands are of particular interest. Among them, the commercially available Ru-Macho® reveals the conversion of atmospheric CO2 to methanol. However, catalytic activity is still low to be applied in industry, and the mechanism for catalytic CO2 hydrogenation is yet to be explored in detail. Here, we hypothesized that utilization of a rigidified pincer system analogous as a Macho-type ligand might solve a metal leaching issue under catalytic conditions because such a ligand can stabilize the active metal site. To test this hypothesis, we have compared a ditolylamine based PNP– (PNP– = bis(2-(diisopropylphosphaneyl)-4-methylphenyl)amide) and a rigidified acridane based PNP ligand, acriPNP– (acriPNP− = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide) respectively to accommodate a Ru(II) center and explored the catalytic activity of the resulting complexes for the hydrogenation of CO2. In this study, we will present synthesis and characterization of (acriPNP)RuII(CO)(H)(PPh3) and (PNP)RuII(CO)(H)(PPh3) (1 and 1') as our homogeneous catalysts. Complex 1 and 1' were synthesized by the metalation of (acriPNP)Li(THF) and (PNP)Li(THF) with RuII(CO)(Cl)(H)(PPh3)3. Further treatment of 1 and 1' with Li(Et3BH) generated the divalent dihydrido ruthenium species [Li][(acriPNP)RuII(CO)(H)2] (3) and [Li][(PNP)RuII(CO)(H)2] (3'), which is an important intermediate of the catalytic reaction. Upon addition of CO2(g), 3 and 3' was immediately converted to 5-coordinate (acriPNP)RuII(CO)(H) (5) and (PNP)RuII(CO)(H) (5') along with the generation of Li(OCHO) as a precipitant. By adding tetrabutylammonium formate ([TBA][OCHO]), the corresponding formate complexes, [TBA][(acriPNP)RuII(CO)(H)(OCHO)] and [TBA][(PNP)RuII(CO)(H)(OCHO)] (4 and 4') were generated and analyzed. Additional steps involve further reduction of formate to give methanol. All steps were compared with the previously known mechanism for the Ru-Macho® system as a benchmark model.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-66**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

One-Step DNA Functionalization of Metal-Organic Framework Nanoparticles

<u>Hyojung Kang</u>, So-Jung Park*

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

Due to their large surface area, high stability and structural diversity, metal-organic frameworks (MOFs) have great potential in many applications such as gas storage, catalysis, sensing and drug delivery. For the bio-application of MOFs, biocompatible ligands such as DNA, peptides, the hydrophilic polymer etc. ligands are necessary. DNA is one of the versatile ligands due to its addressability and biocompatibility. Several methodologies have been reported thus far for DNA functionalization of MOF. However, previous DNA functionalization methods demand the chemical modification of organic linkers of the MOF, which introduces synthetic challenges. In this study, we report a one-step DNA functionalization method for different types of Zeolitic imidazolate frameworks (ZIFs), which have 2-methylimidazole (2-mim) as the organic ligand. We have exploited the typical N-alkylation reaction between 2-mim and bromine-modified DNA, which allows for the direct functionalization of MOF. The recognition properties of the DNA on the surface of the MOF have been verified by testing the hybridization efficiency and melting behavior. The stability analysis confirms the increased stability of the MOF functionalized using this technique when compared with that of the other reports. This methodology offers a simple one-step DNA functionalization of MOF which does not require tedious multiple synthetic steps.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-67**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Enhanced drug loading efficiency and long-term drug release based on porous silicon nanoparticles via self-sealing chemistry of calcium/magnesium silicate

Jaehui Lee, Dokyoung Kim[1,*]

Department of Precision Medicine, Kyung Hee University, Korea
[1]*College of Medicine, Kyung Hee University, Korea*

Porous silicon nanoparticles(pSiNP) offer numerous advantages including biocompatibility, high drug loading efficiency, the ability for surface modification in targeted drug delivery. So they are widely studied in the biomedical field. However, the drug delivery effect of pSiNP is reduced due to their easy degradation in biological media.In this study, we prepared a novel nano-formulation based on pSiNPs (Ca/Mg-pSiNP) that self-seals calcium ion (Ca2+) and magnesium ion (Mg2+) improve these limitations. Ca/Mg-pSiNPs are formulations with high drug loading efficiency and slow release rates as compared to previously reported. Profiling the release of loaded drugs(mitriptyline and duloxetine) on Ca/Mg-pSiNP resulted in more consistent drug release curves compared to the as-prepared pSiNP. This work provided a novel pSiNP formulation that effectively controls sustained drug release and propose it as an advanced drug delivery system.

Poster Presentation : **INOR.P-68**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Zn and Cu substitution on the Electronic Structure and Thermoelectric Properties of the $Ca_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu) System

Junsu Lee, Tae-Soo You[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

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. 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) 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^{2+}, 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), but rather $A_9Cd_{4.5-x}M_x$Sb9 (M = Zn and Cu)—a distinct structure compared to the previously established $A_9M_{4.5}Sb_9$ (A = Ca, Yb, Eu, Sr; M = Zn, Mn) structure. A series of compounds in the $Ca_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu; x =0.45, 1.35) 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; x =0.45, 1.35) were thoroughly examined.

Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Double-doping Effect of the Zintl Thermoelectric $Ca_{3-x}Sr_xAl_{1-y}Zn_ySb_3$ System

Dong Hwan Seo, Tae-Soo You[1,*]

Chungbuk Natioanl University, Korea

[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Thermoelectric(TE) materials and devices have been considered one of the solutions for global warming crisis they can directly convert wasted heat generated by different heat sources into electricity. The measure of a thermoelectric material's efficiency is represented by the value of zT, which is calculated as $zT = \alpha^2\sigma T / (\kappa_e + \kappa_l)$, where α is the Seebeck coefficient, σ is the electrical conductivity, T is the operating temperature, κ_e is the thermal conductivity contribution from electrons and holes transporting heat, and κ_l is the thermal conductivity contribution from phonons traveling through the lattice. Zintl is a highly valued thermoelectric material due to its complex bonding structure, which consists of covalently bonded anionic sub-structures within a lattice of electropositive cations, resulting in a high zT value.The Zintl phase thermoelectric compounds in the A_3MPn_3 (A = Ca, Sr, Ba, Eu ; M = Al, Ga, In; Pn = Sb, As, P) system has been reported to have five different structure types, including orthorhombic Ca_3AlAs_3(*Pnma*), Ba_3AlSb_3(*Cmce*), Ba_3GaSb_3(*Pnma*) and monoclinic Sr_3GaSb_3($P2_1/c$), Rb3TiO3($P2_1/c$). Among these, Ca_3AlSb_3 stand out with its Ca_3AlAs_3 structure type(Ca type) and is composed of infinite chains of corner-sharing $AlSb_4$ tetrahedra. Ca type structures exhibit remarkably low thermal conductivity due to their intricate architectures and also exhibit P-type thermoelectric properties, a trait substantiated through both Density Functional Theory (DFT) calculations and measurements of the Seebeck coefficient.The synthesis of Zintl $Ca_{3-x}Sr_xAl_{1-y}Zn_ySb_3$ induced lowered the thermal conductivity through the size difference between the two ions. In addition, Al was doped with Zn to increase the p-type characteristics to induce better physical properties. These compounds were synthesized using arc-melting method and Pb-flux method, and their crystal structures were characterized using powder and single-crystal X-ray diffractions. It was found that the crystal volume increased as larger amounts Sr were added, as confirmed by single-crystal X-ray diffraction data.The electronic structure of the title compounds was studied using theoretical calculations with the TB-LMTO method, and the resulting density of states (DOS) and band structure were analyzed in detail. Subsequently, the physical properties of the samples were measured using Seebeck and electric resistivity measurements.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-70**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Cation Substitution for the Electronic Structure and Thermoelectric Properties of the $Ba_{1-x}Eu_xZn_2Sb_2$ System

Daewon Shim, Tae-Soo You[1,*]

Chungbuk Natioanl University, Korea

[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Nowadays, with global warming and abnormal climate becoming serious, the seriousness of energy problems is emerging. Thermoelectric materials can be a solution to the energy problem in modern society. Among the various thermoelectric materials, the Zintl phase can be considered one of the best candidates. Recently, the AM_2Pn_2 (A = Ca, Sr, Ba, Eu; M = Mn, Zn, Cd; Pn = P, As, Sb, Bi) series has been extensively investigated as Zintl phase thermoelectric material, and the three major structure types have been identified: the $ThCr_2Si_2$-type having metallic behavior, the $CaAl_2Si_2$-type and the $BaCu_2S_2$-type both showing the semiconducting behaviors. To investigate the effect of the Eu substitution for the crystal structure with semiconducting characteristic, Series of $Ba_{1-x}Eu_xZn_2Sb_2$ ($0.04(1) \leq x \leq 0.15(1)$) have been successfully synthesized by both the Nb-tube and molten Pb-flux method. The reactions produced large bar-shaped single crystals, and their isotypic crystal structure was characterized by the powder and single-crystal X-ray diffraction analysis. Based on the X-ray diffraction results, the unit cell volumes surely decrease as the amount of relatively smaller Eu increases. To understand the electronic structure of the title compounds, a series of theoretical calculations using the hypothetical $Ba_{0.5}Eu_{0.5}Zn_2Sb_2$ model was performed by the tight-binding linear muffin-tin orbital method, and the resultant DOS and COHP curve analyses were thoroughly investigated. By mixing Eu at the Ba-site, a DOS curve shifted toward the more metallic property. The thermal conductivity, electrical conductivity, and Seebeck coefficient of $Ba_{1-x}Eu_xZn_2Sb_2$ ($0.02 \leq x \leq 0.15$) were also carefully studied. Lowest thermal conductivity of 0.54 W/m·k is obtained for $Ba_{0.92}Eu_{0.08}Zn_2Sb_2$ sample at 563 K. The highest *ZT* of

ca. 0.39 is obtained for the $Ba_{0.92}Eu_{0.08}Zn_2Sb_2$ sample at 697 K. In addition, the expected highest *ZT* is *ca.* 0.53 at 749 K in $Ba_{0.98}Eu_{0.02}Zn_2Sb_2$.

Poster Presentation : **INOR.P-71**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Synergistic Effects of Cation Substitution and *p*-type Doping for Thermoelectric Materials: the $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ System

Naeun Seo, Tae-Soo You[1,*]

Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Thermoelectric (TE) materials are materials capable of generating electricity by using a temperature difference. The development of TE materials with efficient physical properties can convert wasted heat into electricity, thereby may solve the problem of global warming. TE materials can be made using the Zintl phase, which is easy to dope because of its semiconductor properties and complex crystal structure. Recently, the Zintl phases $A_9M_4Pn_9$ (A = Ca, Yb, Eu, Sr; M = Zn, Mn) system has been studied to improve the TE properties by regulating the contents of Zn. A previous study proposed that the maximum *ZT* value reached 1.1 in the $Ca_9Zn_{4.6}Sb_9$ system. Studies have been conducted on the 9-4-9 system, which adjusted the Zn ratio to 4.5 to stabilize the overall charge. To make a new attempt, the experiment was designed to increase electrical conductivity by mixing Yb^{2+} utilizing the relatively high electronegativity of Yb. As a result, it was confirmed what kind of change in TE properties occurs due to differences in electronegativity. Further, by adding a *p*-type dopant to mix Cu^+ with Zn^{2+}, not only did the effect of Ca/Yb mixing, but also the hole carrier concentration increased to obtain an overall synergistic effect.

A series of compounds in the $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ ($0.5 \leq x \leq 4.5$; $0.05 \leq y \leq 0.15$) system was synthesized by the molten Pb-metal flux method, and we obtained the bar-shaped single-crystal with good crystallinity. The crystal structures were characterized by powder X-ray diffractions and single-crystal X-ray diffractions (PXRD and SXRD). The SXRD results substantiated that the Ca3 site with the largest QVAL among the five cation sites is most preferred when replacing Yb. To understand the electronic structure, a series of theoretical calculations using three hypothetical models: $Ca_9Zn_{4.5}Sb_9$, $Ca_8YbZn_{4.5}Sb_9$, and $Ca_8YbZn_4Cu_{0.5}Sb_9$ were performed by TB-LMTO method. Electrical conductivity, Seebeck coefficient, and thermal conductivity were measured to unveil the thermoelectric performance of the three title compounds. With the substitution of Yb, the electrical conductivity improved significantly as phonon scattering and carrier concentration increased. When we proceeded with *p*-doping together, *ZT* increased significantly compared to only the substitution of Yb performed. As a result, the co-doping of Yb and Cu derived a synergistic effect, which greatly improved thermoelectric performance.

Poster Presentation : **INOR.P-72**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Study of Electrochemical Properties of Nano-rod MnS@rGO as High-performance Anode for Lithium-Ion Batteries

Wonbin Nam, Hyerin Yoo[1], Yoon Myung[2], Chan Woong Na[2], Jaewon Choi*

Department of Chemistry, Gyeongsang National University, Korea
[1]*Gyeongsang National University, Korea*
[2]*Korea Institute of Industrial Technology, Korea*

Manganese sulfide (MnS) has been noticed as an anode for lithium-ion batteries due to its high theoretical capacity (616 mAh/g) through a conversion reaction, low cost, and eco-friendliness. Nevertheless, some problems persist, such as low cycle stability caused by volume expansion and poor electronic conductivity. Using the one-pot method, this work prepared MnS nanoparticles grown on reduced graphene oxide (rGO). rGO serves to improve electronic conductivity and protect against the aggregation of nanoparticles. The as-prepared MnS and MnS@rGO powders were conducted by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). MnS nanoparticle's size is around 40 nm, and the particles are homogeneously dispersed on the rGO. MnS@rGO nanocomposite exhibited enhanced electronic conductivity and remarkably improved discharge capacity of 624 mAh/g after 100 cycles, compared with bare MnS nanoparticles, at a current density of 500 mA/g. Thus, MnS@rGO composites are expected to be a promising alternative for anode materials in lithium-ion batteries (LIBs).

Poster Presentation : **INOR.P-73**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Electrochemical Properties of hexagonal structure type of SnS_2@rGO as Anode materials for Lithium-Ion Batteries

Hyerin Yoo, Wonbin Nam, Chan Woong Na[1], Yoon Myung[1], Jaewon Choi*

Department of Chemistry, Gyeongsang National University, Korea

[1]*Korea Institute of Industrial Technology, Korea*

SnS_2-based materials are one of the most promising anode materials for lithium-ion batteries due to their unique two-dimensional layered structure, impressive theoretical capacity, and alloy metal properties. However, SnS_2 suffers from low cycle life stability and large volume expansion during the charge/discharge process. To solve these problems and enhance performance, we composed carbonaceous materials, such as reduced graphene oxide(rGO). We comprehensively analyzed the SnS_2@rGO composites using SEM, XRD, XPS, and TEM techniques. It was found that the composites of SnS_2 nanoplates and rGO nanosheets are closely coupled, providing efficient paths for electrons/ions to ensure high electrical conductivity and sufficient buffer space to alleviate volume expansion. The SnS_2@rGO nanocomposite demonstrated enhanced cycling stability and discharge capacity, as evidenced by electrochemical testing (700 mAh/g at 100 mA/g after 100 cycles; 317.9 mAh/g at 1000 mA/g after 200 cycles). This research will facilitate the development of diverse energy storage materials based on SnS_2

Poster Presentation : **INOR.P-74**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Design of CMOF by PSM method for Enantiomer Separation

Seokjin Noh, Jin Yeong Kim[1,*]

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

Enantiomer molecules show great difference on performance in pharmaceutical, analytical industry, but obtaining enantiomer pure molecules remains a challenging problem because of their similar physical and chemical properties. For high efficiency of enantiomer separation, developing an efficient separation system which have high surface area and high density of chiral interaction site is a key factor. Chiral Metal Organic Frameworks (CMOFs) provides high density of chiral site, which makes them promising material for enantiomer separation. Yet, MOFs are generally synthesized as crystalline powder form, separation efficiency are reduced due to their large non-selective void between particles. Here in, we reported CMOF gels which have a small particle size and high density of chiral site, making CMOF gels promising packing material for enantiomer separation. We prepared CMOF gel via PSM of an achiral MOF gel by introducing chiral molecule. Crystallinity and successful PSM of CMOF gel were characterized by Powder X-ray diffraction (PXRD), infrared(IR) spectroscopy, and Nuclear Magnetic Resonance(NMR) Spectroscopy. Particle size was observed via Scanning Electron Microscopy (SEM). To confirm separation efficiency through liquid chromatography, MOF was packed into an LC Column, and enantiomer selectivity was measured.

Poster Presentation : **INOR.P-75**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Facile and Naked-eye Decoding of Hydrohalic Acids using Metal-Organic Frameworks

Wonhyeong Jang, Jin Yeong Kim*

Department of Chemistry Education, Seoul National University, Korea

Acids are widely use in laboratory and industrial fields. However, direct exposure to or inhalation of acids can lead to burns, respiratory distress, lung injury, and even fatalities. When working with acids, mislabeling or the absence of labeling could potentially result in an accident if different types of acids are mixed or if acids are combined with organic solvents. Thus, it becomes important to accurately distinguish between various acid types and employ them appropriately. Herein, we report a facile and naked-eye decoding system of hydrohalic acids using copper-coordinated MOF-808-EDTA. When copper-coordinated MOF-808-EDTA exposures to vaporized hydrohalic acid, its color changes to different color, which can be readily decoded by naked-eye within minutes without compromising the integrity of the framework. In detail, six-coordinate Cu-EDTA complex was grafted on the MOF-808 framework, ensuring a high density of sensing sites that enables for direct exposure to vaporized acid. Upon contact of the Cu-EDTA complex with vaporized acid, EDTA undergoes protonated and copper ion released to yield four-coordinate Cu-halide species simultaneously, confirmed by using FT-IR spectroscopy, X-ray photoelectron spectroscopy, and UV-Vis-NIR spectroscopy. Cu-halide species exhibit distinct colors, enabling easy naked-eye decoding of hydrohalic acid with MOF-808-EDTA system. Furthermore, the framework can be regenerated to its pre-exposure state by subjecting it to heat within an hour. This regenerated framework can then be reused for detecting previously identified acids or other hydrohalic acids. This research can extend to enhancing safety measures and averting accidents in diverse domains involving acid utilization.

Poster Presentation : **INOR.P-76**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Tunable emission in metallo-supramolecular gels

Eungyu Lee, Hyeon Min Han[1], Sung Ho Jung[1,*], Jong Hwa Jung[1,*]

Gyeongsang National University, Korea

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

We have developed a tunable emissive metallo-supramolecular gels functionalized with lanthanide coordination bonds using a low molecular weight gelator 1(LMWG) having terminal terpyridine with amide. In the presence of TbIII and EuIII ions, lanthanides coordination to a gelator 1 results in green and red emissive supramolecular gels, respectively. These gels (1-Tb and 1-Eu) showed nanofiber morphology. Furthermore, temperature-dependent absorption spectra changes of the 1-Tb display a sigmoidal transition, indicating that the growth of aggregates during gel formation occurs via an isodesmic self-assembly mechanism.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-77**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

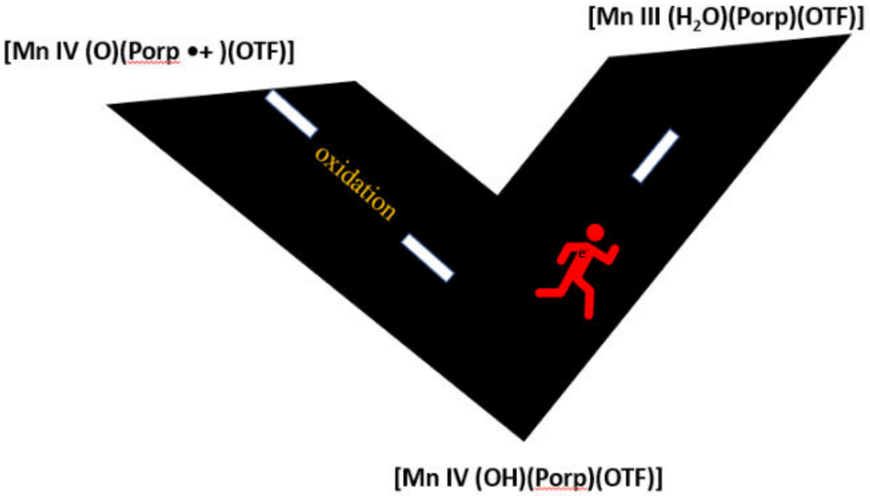
Disproportionation reaction- A DFT Study.

Steiny Russelisaac Premakumari, Kyung-Bin Cho[1,*]

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

Density Functional Theory DFT) calculation were performed to study the disproportionationreaction of high-valent MnO species (2× [Mn IV (O)(Porp)] → [Mn IV (O) (Porp •+)] + [Mn III (O)(Porp)], Porp = porphine 2-), which experimentally occurs (only) in the presence of acid.[1] Energy calculations of all possible derivatives of the above species with regards to protonation and OTF axial ligation enabled us to calculate the thermodynamics of the reaction, and pinpoint the exact protonation and chlorination state of each of the reactant and product compounds.[2] Thus, we predict that the real disproportionation reaction occurring is a proton coupled electron transfer reaction forming water, 2× [Mn IV (OH)(Porp)(OTF)] → [Mn IV (O)(Porp •+)(OTF)] + [Mn III (H 2 O)(Porp)(OTF)].[3] Furthermore, knowing the preferred spin state for each of the compounds lead us predict that the most likely electronic state for the reactant and product complexes are antiferromagnetically coupled singlets.[4] This in turn enables us to pinpoint the exact orbitals the electron is transferred from/to. The current study is an example where relatively rudimentary calculations can give surprisingly deep insights into a biochemically important reaction.Reference1.Chen, J.; Yao, J.; Li, X.-X.; Wang, Y.; Song, W.; Cho, K.-B.; Lee, Y.-M.; Nam, W.; Wang, B., Bromoacetic Acid-Promoted Nonheme Manganese-Catalyzed Alkane Hydroxylation Inspired by α-Ketoglutarate-Dependent Oxygenases. ACS Catalysis 2022, 12 (11), 6756-6769.2.Mpidi Bita, H.; Huber Johannes, A. J.; Palma, P.; Tannert, T., Prevention of Disproportionate Collapse for Multistory Mass Timber Buildings: Review of Current Practices and Recent Research. Journal of Structural Engineering 2022, 148 (7), 04022079.3.Nam, W., High-Valent Iron(IV)–Oxo Complexes of Heme and Non-Heme Ligands in Oxygenation Reactions. Accounts of Chemical Research 2007, 40 (7), 522-

531.4.Yang, B.; Yao, H.; Yang, J.; Chen, C.; Shi, J., Construction of a two-dimensional artificial antioxidase for nanocatalytic rheumatoid arthritis treatment. Nature Communications 2022, 13 (1), 1988.



Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis of titanium using [N, O] type ligands including azole, and cyclic addition and copolymerization reactions using carbon dioxide

Jungwi Mok

chemistry, Chonnam National University, Korea

Due to various abnormal climates, countries around the world recognize the seriousness of environmental pollution and announce carbon neutrality. As a means of carbon neutrality, several CCUS technologies are advancing. The synthesis of aliphatic polycarbonate through the copolymerization of CO2 and epoxide by Inoue et al in the 1960s is currently considered one of the most feasible and useful technologies among many CCUS technologies. Our laboratory previously reported titanium tetrazole complexes by converting FI catalysts, which are widely used in olefin polymerization. In this study, titanium complexes of various azoles such as Pyrazole and Triazole were synthesized. For the synthesized titanium composite, the cycloaddition reaction and copolymerization reaction of PO and CHO were attempted. The difference in crystallographic structure and the change in catalyst activity due to the change in the number of N in azole were studied.

Poster Presentation : **INOR.P-79**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Intersection of Apoptosis and Ferroptosis Cell Death Pathway Confirmed by RNA Sequencing Analysis : Eruptive Generation of Hydroxyl Radical in Gastric Cancer

Hyungbin Park, Chaewon Ahn[1], Yougang Kim[2], Yerin Lee[3], Seungwoo Hong[*]

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

[1] Department of Chemistry, Sookmyung Women's University, Korea

[2] Chemisty, Ewha Womans University, Korea

[3] Chemistry & Nanoscience, Ewha Womans University, Korea

Gastric cancer (GC), is the 5th most common cancer worldwide, particularly in eastern asia (Mongolia, China, Japan and Korea). GS is still a problem because it has a very fast growth rate and metastasis, thereby, it is difficult to treat it. Recently, the new programmed cell death, ferroptosis, accompanied by a large amount of iron accumulation and lipid peroxidation during the cell death process have emerged as a novel strategy to treat cancers. Herein, we synthesized nonheme metal complexes bearing N2Py3OH ligand (2-((2-(bis(pyridin-2-ylmethyl)amino)ethyl)(pyridin-2-ylmethyl)amino)ethanol). They were characterized by various spectroscopic techniques such as UV−vis spectroscopy, cyclic voltammetry and electrospray ionization mass spectroscopy (ESI-MS). We confirmed that the H2O2 activation by iron complex occurred via Fenton-like reaction and hydroxyl radical was quantitatively generated. When the iron complex incubated in gastric cancer cells (MKN28, MKN45 and AGS), it has ability to induce ferroptosis by catalyzing Fenton-like reaction in cancer cells; higher concentrations of ROS in intracellular networks lead to ferroptosis. The presence of iron complex enhanced GPX4 depletion and hydroxyl radical formation. Appoptosis-Ferroptosis hybrid pathway were identified using RNA sequencing analysis and Western blot experiments.

Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

High-Performance Lithium Metal Batteries Enabled by Nanodiamond Scaffolds

Jaeseong Kim, Haksung Jung[1,*], Won Cheol Yoo[*]

Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea

[1]*Quantum Technology Institute, Korea Research Institute of Standards and Science, Korea*

Lithium metal batteries (LMBs) have attracted great attention due to their outstanding theoretical capacity of 3,890 mAh g-1 but the formation of persistent lithium dendrites during cycling remains a challenge. In this study, we present nanodiamonds as a scaffold for ultra-stable LMBs. Mechanically robust and lithiophilic nanodiamonds successfully mitigated dendrite formation, thereby exhibiting outstanding long-term stability and notably low overpotential values at various current densities.

Poster Presentation : **INOR.P-81**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Tailoring the morphology of WO_x nanoparticles for near-infrared absorbing polymer-ceramic composite fiber

Seo Young Kang, Yongyeol Park, Young Joon Yoo[1,*], Yuanzhe Piao[2,*], Sang Yoon Park[3,*]

Department of Applied Bioengineering, Seoul National University, Korea

[1]*Advanced Institute of Convergence Technology, Korea*

[2]*Graduate School of Convergence Science and Technol, Seoul National University, Korea*

[3]*Electronic Engineering, Kyonggi University, Korea*

The near-infrared (NIR), spanning 800-2500 nm in wave length, is a key area in solar energy utilization, constituting around 50% of the solar energy spectrum. NIR selective absorbers enable diverse solar-thermal applications, managing NIR-generated heat while preserving color and transparency in the visible region. There are various utilization examples. One of them is the smart window with NIR-selective absorber coatings, maintaining transparency while blocking NIR to decrease indoor temperature and cooling energy consumption. Embedding NIR-selective absorber particles in polymer fibers to use NIR as a heat source for Personal Thermal Management is another example. Tungsten oxide has attracted attention as an effective NIR absorber due to its selective absorption in the NIR range through bandgap engineering achieved via doping or oxygen vacancies. Various synthesis methods propose Tungsten oxide-based NIR absorbing nanoparticles in forms of sphere, plate, rod, and wire, yet in applications, predominant choice is spheres. Despite the significant influence on the mechanical properties in textile, comprehensive studies addressing the optical and mechanical properties of NIR absorbing particle embedded polymer fibers based on particle morphology are still lacking. Our study employs hydrothermal and solvothermal methods for diverse tungsten oxide nanoparticles morphologies. H_2 gas reduction enhance NIR absorbance through oxygen vacancies. Prepared nanoparticles are embedded in polymer solution and produce fibers by wet spinning process. These fibers are analyzed to evaluate

mechanical properties and photothermal efficiency. Our aim is to identifiy advantageous morphologies for producing textiles with various colors, suitable for the winter.

Poster Presentation : **INOR.P-82**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Converting Achiral to Chiral Metal-Organic Framework for Asymmetric Diels-Alder Reactions

Hyeonsu Kim, Younghu Son[1], Purna Chandra Rao[1], Jeong Yera[1], Sunggi Lee[2,*], Minyoung Yoon[1,*]

Department of ChemistryDepartment of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

[1]*Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea*

[2]*Dept. of Physics and Chemsitry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Metal-organic frameworks (MOFs) with high surface areas and thermal stabilities are applied in various fields, such as heterogeneous catalysis, gas storage and separation, and chemical sensors. Among these MOFs, research on chiral MOFs, which provide unique platforms due to their chirality, has also attracted much attention. The synthesis of chiral MOFs generally uses direct methods and post-synthetic modifications. However, these methods are difficult to apply because it is challenging to synthesize a new chiral ligand, or the ligands can be easily leached out. Because of the difficulty in synthesizing new chiral MOFs, this research field is fading out. In this study, we present the preparation of chiral MOFs through solvent-assisted ligand incorporation (SALI). This method allows facile preparation of chiral MOFs with a strongly bound chiral moiety as a building block of the MOF. Herein, L-proline was introduced into the MOF-808 using SALI methods to convert an achiral MOF (MOF-808) to a chiral MOF (MOF-808-SALI). We compared the catalytic activity of a chiral MOF and an achiral MOF in asymmetric Diels-Alder reactions with investigating the difference in enantioselectivity. Both chiral and achiral MOFs showed similar conversion (>90%) for the reaction between isoprene and maleimide derivatives. The catalytic site of achiral Zr-MOF is a Lewis acidic site, whereas the chiral Zr-MOF has an additional catalytic site, L-proline, which may induce enantioselectivity in asymmetric Diels-Alder reactions. Furthermore, we plan

to investigate the size effect using chiral MOFs depending on the size of the starting material through maleimide derivatives.

Poster Presentation : **INOR.P-83**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Trinuclear Ruthenium Complexes: Catalyzing Photocatalytic Oxidation for Biomass-Derived HMF Conversion

Yerin Lee, Chaewon Ahn[1], Yougang Kim, Hyungbin Park, Seungwoo Hong*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea
[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Diminishing fossil fuel reserves and increasing concerns about global warming suggest that the development of sustainable energy sources will be necessary in the future. The conversion of biomass, which is organic matter used as a renewable energy source, into high-value-added chemicals presents a promising strategy for addressing environmental problems. The selective oxidation of 5-hydroxymethylfurfural (HMF) derived from biomass into 2,5-furan dicarboxylic acid (FDCA) holds particular appeal as an attractive reaction. This is because FDCA can serve as a monomer for synthesizing polymers with fewer CO_2 emissions. Herein we report a heterogeneous photocatalyst $[Ru_3(\mu_3\text{-}O)(OAc)_6L_3]^+$ (L = py, Mepy, $N(CH_3)_2$py, CNpy, Clpy, quinoline, isoquinoline). We have confirmed the photocatalytic reaction tendencies of these compounds using various spectroscopic methods such as UV-vis, Electrospray Ionization Mass Spectroscopy (ESI-MS), and X-ray Diffraction (XRD). Our findings indicate that compounds tend to exhibit improved photocatalytic oxidation of HMF when an electron-withdrawing group is attached. This work unveils possibilities for HMF as a biomass since it has discovered a catalyst that effectively performs photocatalytic oxidation for converting HMF to FDCA.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Modulating Polariton Lasing Properties by Controlling Gain Volume in the Fabrication of Multi-Layered Axial Heterostructure Nanorods

Huiyeong Kang, Minji Ko, SeungJe Lee, Seonghyun Jeong[1], Jae Kyu Song[1,*], Young rag Do[*]

Department of Chemistry, Kookmin University, Korea

[1]*Department of Chemistry, Kyung Hee University, Korea*

Nanorods with a multi-layered axial heterostructure were fabricated to enable polariton lasing. The primary objective encompassed the induction of polariton lasing with the aim of acquiring modifiable attributes. These attributes encompassed the lasing threshold, emitted light wavelength, and mode spacing. To fabricate these nanorods, a top-down fabrication approach was employed, with exact layering of InGaN, GaN, and AlGaN films via the MOCVD technique, resulting in a precisely stacked structure. Cylindrical GaN nanorods were meticulously cut to achieve nearly uniform lengths (~3µm) and diameters (~500nm) with flat ends. Amplification efficiency and charge carrier transfer variations lead to distinct lasing features in the heterostructure. Adjusting the layer thickness allows tuning of the mode spacing as polaritons in different layers experience varying refractive indices. The effective index of GaN amplifies the contrast in indices at the interface, leading to enhanced reflectivity and a lowered lasing threshold. The distinctive Fabry-Perot lasing modes offer adjustable mode spacing through manipulation of polaritonic effects and composite materials. The addition of silver metal thin films on the terminal surfaces enhances reflectivity, thereby allowing regulation of the lasing threshold. The first-ever detection of polariton lasing in a multi-layered axial heterostructure nanorod underscores the potential to manipulate lasing characteristics through modifications of the gain volume, layer arrangement, and end facet configuration. Consequently, the occurrence of polariton lasing with multiple colors within the multi-layered heterostructure suggests the potential for adjustable lasing attributes, including wavelength, threshold, and mode spacing, through manipulation of the gain volume, layer arrangement, and end facet design. Leveraging these manageable lasing features, polariton nanolasers hold promise for boosting the performance of nanoscale devices.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-85**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

The fabrication of a GaN-based micro-light-emitting diode (LED) and fluidic self-assembly using low frequency sonication

Young rag Do*, Yong Jae Lee, SeungJe Lee, Huiyeong Kang, Yun Jae Eo

Department of Chemistry, Kookmin University, Korea

This study investigates the production process of GaN-based micro-LED arrays and LED chips, which are separated using laser dicing. Micro-LEDs were transferred to Si cartridges using fluidic self-assembly with low-frequency sonication. Indium tin oxide (ITO) was deposited onto GaN, which was grown on a 4-inch patterned sapphire substrate (PSS). Lateral LED arrays were fabricated through a series of photolithography, etching, and deposition processes. We measured the electroluminescence spectrum and I-V curve by using a probe station from 0.1mA to 50mA. We believe that properly aligned GaN-based LED chips, using suitable transfer technology, will have wide-ranging applications in the display industry.

Poster Presentation : **INOR.P-86**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Amine decorated (Zn, Zn)-bimetallic catalyst for the valorization of carbon dioxide

Ho Jun Lee, Jungseok Heo*

Department of Chemistry, Chungnam National University, Korea

The rapid increase in carbon dioxide emissions over the past few decades has led to significant environmental issues related to global warming. As a result, research is being conducted on technological solutions to effectively reduce carbon dioxide emission. This study focuses on the innovative development of catalysts for carbon dioxide conversion, presenting the noble design, synthesis, and conversion reactions of the bimetallic catalyst. The development of efficient catalysts, using zinc, magnesium, and other materials instead of cobalt and nickel as central metals. This approach demonstrates the potential to minimize the cost and difficulty of carbon dioxide conversion reactions.We also studied on a cage-type catalyst to compare with an open-type catalyst in terms of catalytic activities. We will present details regarding relationship of the catalyst structure design and their efficiencies in carbon dioxide conversion reactions.

Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Balancing the Imbalance: Design Strategies for Heterobimetallic Metallohelicates

Kyunghwan Min, Heechan Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Dinuclear metal complexes, reminiscent of those present in metalloenzymes, have long captured scientific attention due to their capability of performing exceptional catalytic reactions. The synthesis of such dinuclear species, however, presents a formidable challenge. This complexity arises primarily from the need for the supporting ligands to satisfy a precise degree of steric constraints, so that the formation of undesirable polynuclear clusters or mononuclear complexes is suppressed. In our approach, strategic modifications were made on the tridentate bis(benzimidazolyl)pyridine ligand core by appending methyl and pyridyl groups. This molecular design enforces the pentadentate ligand L to adopt a distinct bimetallic helicate configuration, denoted as $[M_2L_2]^{4+}$. We also found that the installation of alkyl groups at the benzimidazole nitrogen atoms aid the exclusive formation of bimetallic helicate structure. X-ray crystallographic analysis revealed an uneven distribution of ligand donor atoms: one metal ion is supported by six *N*-donors, whereas the other is coordinated by four *N*-donors, leaving *cis*-divacant sites occupied by solvent-derived monodentate ligands. Such geometric configuration could potentially be harnessed for heterobimetallic catalysis. This presentation will articulate our strategic design, progresses in the synthesis, and future research directions in heterobimetallic helicates.

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Moisture-Triggered Proton Conductive Switch in Metal-Organic Frameworks : Role of Coordinating Solvents

HongKyu Lee, Dohyun Moon[1,*], Min Kim[2,*], Dae Woon Lim[3,*], Hoi Ri Moon[4,*]

Chemistry, Ulsan National Institute of Science and Technology, Korea

[1] *Beam Operation Team, Pohang Accelerator Laboratory, Korea*

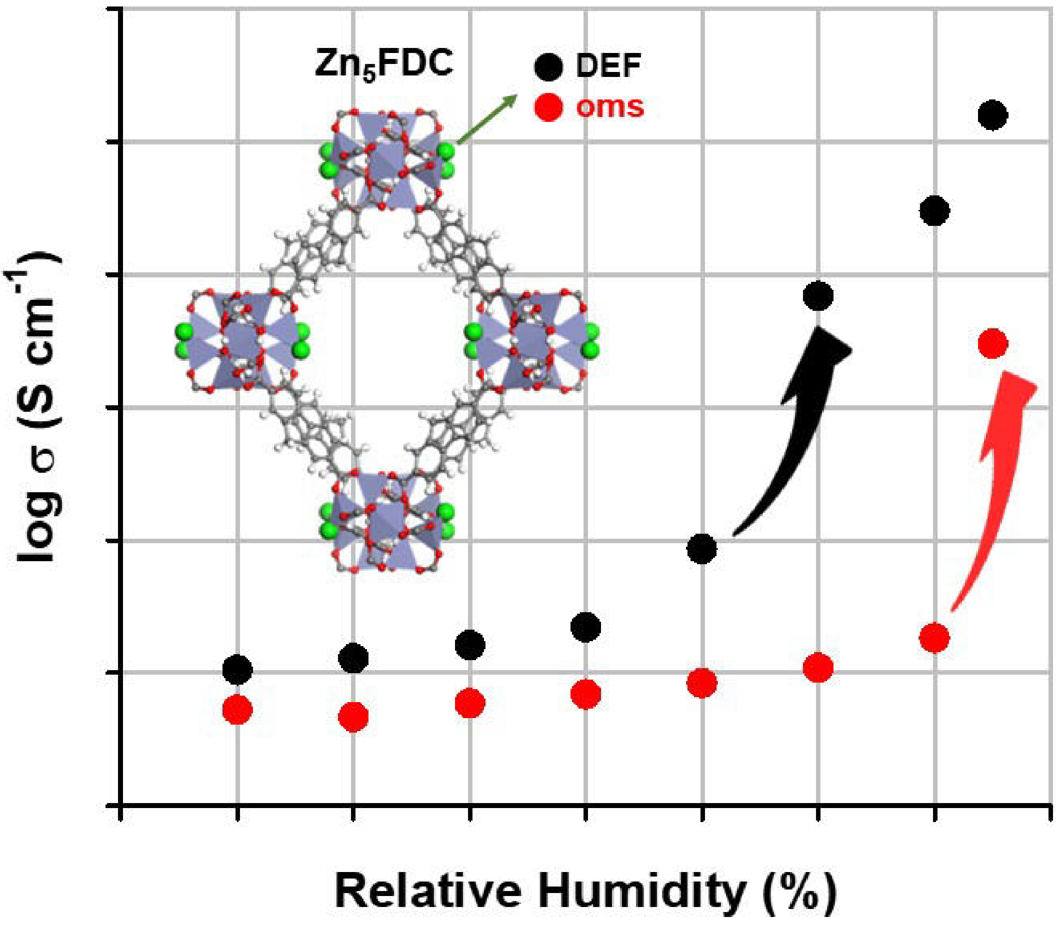
[2] *Department of Chemistry, Chungbuk National University, Korea*

[3] *Department of Chemistry and Medical Chemistry, Yonsei University, Korea*

[4] *Department of Chemistry and Nanosciecne, Ewha Womans University, Korea*

To elucidate the mechanisms of proton conduction, metal-organic frameworks (MOFs), which offer designable metal nodes and organic linkers, have been employed as effective research platforms. In this study, we report the behavior of Zn5FDC, [Zn5(μ3- OH)2(FDC)4], whose proton conductivity and its switching point vary depending on the presence of the coordinating solvents. Zn5FDC with coordinating solvent molecules, [Zn5(μ3- OH)2(DEF)2(FDC)4] (Zn5FDC-DEF), can be synthesized in N,N-diethylformamide (DEF), and even under harsh activation condition coordinating DEF molecules are not removed from the secondary building units (SBUs). Interestingly, [Zn8O3(FDC)4](H3O)4] (Zn8FDC) can be transformed to result in Zn5FDC without coordinating solvent molecules, Zn5FDC-oms (oms = open metal site), by solvent exchange with dichloromethane (DCM) and activation. Comparison of proton conductivity measurements in Zn5FDC-DEF and Zn5FDC-oms under humidity shows the effect of coordinating molecules on proton conduction in MOFs. Both MOFs showed proton conductivity switching phenomenon, but it was occurred in Zn5FDC-oms at relatively higher relative humidity compared to Zn5FDC-DEF (Figure 1). This behavior might be attributed to the structural differences of Zn5FDC with and without coordinating solvent molecules, because Zn5FDC-DEF and Zn5FDC-oms have different structures of SBUs generated by different coordination geometry. In Zn5FDC-DEF, proton conductivity can be induced by coordinating molecule exchange from DEF to H2O molecules in SBUs.

However, since Zn5FDC-oms already has the stabilized structure without the coordinating molecules, approach and coordination bond formation of H2O molecules on the oms requires more energy, as confirmed through geometry optimization. Upon the proton conductivity measurement in moisture, both MOFs converge in the same structure, Zn5FDC-H2O. A cycling experiment in Zn5FDC-H2O at relative humidity 95% and 60 °C reveals the consistent super protonic conductivity, 4.27 x 10–4 S cm–1, retaining its structure.



Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

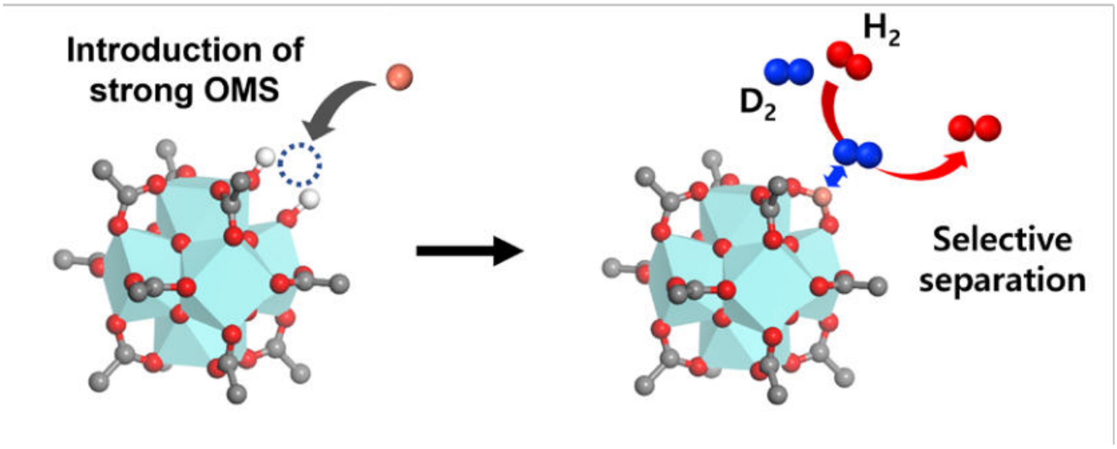
Introduction of Strong Open Metal Sites into Zr-based MOFs for Hydrogen Isotope Separation using CAQS Effect

Jihyun Park, Hoi Ri Moon[1,*]

Chemistry, Ulsan National Institute of Science and Technology, Korea

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

The open metal sites (OMS) within MOFs act as strong binding sites and selectively adsorb guest molecules, which has been used effectively for separation. In particular, Cu(Ⅰ) sites exhibit strong interaction with H2 and π-acidic species through π-backbonding, enabling selective adsorption. In this study, we introduced Cu(Ⅰ) sites into defect sites of three distinct Zr-based MOFs, each with different characteristics. While retaining the crystallinity of MOFs, Cu sites were incorporated and converted to Cu(Ⅰ) state. Notably, in one of the MOFs, the introduced Cu sites were identified as Cu(Ⅰ) state without the reduction process. Calculation of the isosteric heat of adsorption (Qst) for H2 and D2 showed notable values at zero coverage for all three MOFs. Furthermore, the introduced Cu(Ⅰ) sites in these MOFs exhibited distinct Qst values and variations between H2 and D2. This finding suggests the potential for developing efficient separation systems through the comparison of optimized Cu(Ⅰ) sites, utilizing the chemical quantum sieving effect for hydrogen isotope separation.


Introduction of strong OMS
H_2
D_2
Selective separation

Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Optimizing Micro-LED Separation with Electrochemical Etching (ECE) for Enhanced Performance

Young rag Do*, Soyeon Kim, Minji Ko, Yu Jeong Jeong, Yun Jae Eo

Department of Chemistry, Kookmin University, Korea

Organic light-emitting diodes (OLEDs) face challenges such as performance degradation and the "burn-in" phenomenon over time. In contrast, micro-LED technology has emerged as a promising next-generation display solution, offering increased brightness while consuming less power. In this study, electrochemical etching (ECE) was employed as a technique to separate LEDs from a wafer. A 0.3M oxalic acid solution served as the electrolyte, with the GaN wafer connected to the positive electrode (anode). On the other hand, a Pt substrate was connected to the negative electrode (cathode) to apply the necessary voltage for selective porous etching of the n-GaN. Successfully fabricated nanoscale GaN-based dot light-emitting diode (LED) displays with a diameter of 750 nm and a height of 900 nm were achieved. Moreover, the effects of various solvents on separation efficiency, temperature-dependent photoluminescence (TDPL) on the etched wafer, and the overall display performance were examined. The quality of separated LEDs was assessed using scanning electron microscopy (SEM) to detect irregularities or damage that might have occurred during the electrochemical etching (ECE) process. Furthermore, this study opens up possibilities for addressing the challenges associated with micro-LED technology, such as high production costs and material expenses. This investigation explores innovative fabrication techniques and materials to meet the demands of the ultrasmall LED display industry.

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Magnetic Structure Analysis in Water-Coordinated Coordination Polymers

Younghu Son, Yura Seo, Min Jeong Park, Gyungse Park[1,*], Minyoung Yoon[*]

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

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

Coordination polymers (CPs), comprised of metal ions and connecting ligands, have potential as a unique magnet system. These CPs feature multi-dimensional paramagnetic metal chains, especially when they contain transition metal ions like Cr, Mn, Co, and Ni with unpaired electrons. This arrangement leads to ordered electron spins in CPs, resulting in magnetic coupling. The magnetic ordering within CPs enhances or cancels the magnetic moment, while the movement of ions generates electromagnetic fields due to their charge. This interaction between magnetic fields in coordination polymers and electromagnetics from moving ions suggests a correlation between magnetic CPs and conducting ions. CPs with crystallinity, designability, and high density can be one of the candidate materials for providing a unique platform to study magnetic properties with structure analysis. In this work, we present a magnetic properties analysis through neutron experiments in water-coordinated CPs, $[M(HCO_2)_2(H_2O)_2]_n$, where M = Co(II), Ni(II). Interestingly, when the non-hydrated CPs were exposed to high humidity, unusual structural transformation was observed, transforming into an irreversible hydrated form. We obtained the crystal structure of non-hydrated and hydrated Ni-formate, which was unprecedented. To better understand the magnetic properties of hydrated and non-hydrated CPs, neutron diffraction at variable temperatures has been done at ANSTO and J-PARC. The VT-neutron diffraction data at WOMBAT in ANSTO shows a unique diffraction peak in increasing temperature conditions. It is expected that the adsorbed and/or coordinated water molecules in the CPs affect the spin ordering of the CPs. For the detailed study of magnetic properties in the CPs, we conducted high-resolution neutron

diffraction experiments in J-PARC. Furthermore, we will analyze the magnetic structure of CPs via Rietveld analysis. Details of the NPD analysis results will be presented.

Poster Presentation : **INOR.P-92**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

A Novel Approach to Fabricate InP/ZnSeS/ZnS Quantum Dot-Embedded Alumina Microbeads for Color-by-Blue Displays

Jun Hwan Oh, Minji Ko, Yuna Kwon, Yu Jeong Jeong, Young rag Do*

Department of Chemistry, Kookmin University, Korea

Color-by-blue displays have garnered substantial interest in recent years due to their promising attributes of high luminosity, energy efficiency, and a wide range of color representation. In this study, we propose a novel and sophisticated approach to fabricate InP/ZnSeS/ZnS quantum dot (QD)-embedded alumina microbeads, which serve as the foundation for these displays. InP/ZnSeS/ZnS quantum dots were meticulously synthesized using a one-pot hot-injection method, yielding highly luminescent QDs characterized by narrow emission spectra. To enhance their dispersibility and stability within the alumina microbeads, a hydrophobic ligand was employed to modify the QD surface, facilitating efficient incorporation and integration. Employing a sol-gel methodology for the synthesis of alumina microbeads enabled precise control over their size and morphology, yielding uniform and well-defined structures. During the synthesis process, the InP/ZnSeS/ZnS QDs were effectively embedded into the porous structure of the alumina microbeads, ensuring a homogenous distribution of the quantum dots throughout the matrix. Photoluminescence measurements were performed, revealing the ability to tune the emission colors of the QD-embedded microbeads by adjusting the QD composition, allowing for fine-tuning of the display's color output. The proposed InP/ZnSeS/ZnS quantum dot-embedded alumina microbeads exhibit immense potential for utilization in next-generation color-by-blue displays and lighting devices. The amalgamation of high-performance quantum dots with the porous alumina matrix presents an exciting platform that promises to deliver vivid and efficient color displays, marking a significant advancement in display technology.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Density Functional Theory Study of Tyrosine Radical Formation and Di-tyrosine Cross-linking Catalyzed by Transition Metal Ion And 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 disease1). 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 disease2). 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.reference1) Bush Al, Curtain CC: Twenty years of metallo-neurobiology: where to now? *Eur Biophys J* 2008, 37:241-2452) Al-Hilaly et al. A central role for dityrosine crosslinking of Amyloid-β in Alzheimer's disease, *Acta Neuropath.* Commun. 2013, 1, 83.

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Reactivity of Low-valent Nickel Carbonyl Complexes with Methyl Iodide Supported by an Acridine PNP Ligand Containing Phenyl Moieties

Sanha Park, Yunho Lee*

Department of Chemistry, Seoul National University, Korea

Carbon monoxide is a useful small molecule which can be converted into valuable chemicals such as an aldehyde and acetic acid. Among several industrial examples utilizing CO, Monsanto process has its importance to convert CO into an acetic acid with methanol by a rhodium catalyst. A Rh–C bond is formed and generation of a C–C coupled Rh-acetyl complex follows via CO migratory insertion. In nature, acetyl coenzyme A synthase (ACS) catalyzes a synthesis of acetyl-CoA, CO and a methyl cation. In a catalytic mechanism of ACS, a nickel acetyl intermediate is proposed via C–C bond coupling with CO and the methyl cation. In a paramagnetic mechanism, a Ni(I)–CO moiety has been suggested as an active species to produce the acetyl complex. However, reactivity of the Ni(I)–CO species towards alkyl cation is not well-established relative to the CO migratory insertion of a Ni–C bond. Previously, our group reported the reactivity of the series of nickel monocarbonyl complexes supported by a PNP ligand (PNP– = N[2-PiPr2-4-Me-C6H3]2–) with MeI. Upon addition of MeI to a (PNP)NiCO, the resulting products consist of (PNP)NiI (50%), (PNP)Ni(COCH3) (37%) and (PNP)NiCH3 (13%). In addition, our group reported effects of a rigidified acriPNP ligand by tethering the two aryl rings of ditolylamine with a –C(Me)2– bridge. Here, we present the syntheses and characterization of nickel complexes supported by an acridane adapted acriPNP-Ph ligand with two phenyl groups. The two phenyl moieties within the acridane ligand are added to provide a steric effect at the axial site of the metal center. Monovalent nickel complexes, (acriPNP-Ph)Ni and (acriPNP-Ph)Ni(CO), were synthesized from the chemical reduction of divalent nickel bromide complex (acriPNP-Ph)Ni(Br). Further reduction of (acriPNP-Ph)Ni(CO) generated a zerovalent nickel carbonyl {Na(12-C-4)2}{(acriPNP-Ph)Ni(CO)}. SC-XRD, IR, NMR, and

DFT analyses were carried out to examine the detailed geometrical and chemical properties of the complexes. Finally, results from reactions of the low-valent nickel monocarbonyl complexes with MeI will be discussed.

Poster Presentation : **INOR.P-95**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Interrelations of MMP-2/9 and Metal Ions

Minseo Kim, Areum Yun, Hyuck Jin Lee[1,*]

Chemistry Education, Kongju National University, Korea

[1] *Department of Chemistry Education, Kongju National University, Korea*

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., Mg(II), Ca(II), Fe(III), Cu(II), 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-2/9 is suppressed when the concentration of metal ion is high, especially in the presence of Mg(II) and Cu(II) which have similar radii to Zn(II) in MMP-2/9. 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.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-96**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Development of ethane-selective adsorbent by aminal-linked covalent organic frameworks

Hongryeol Yun, Donggyu Lee[1], Chang Seop Hong*

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

Ethylene (C2H4) is a valuable raw material for wide chemical industrial region. However, ethane (C2H6), a byproduct from the C2H4 producing process has very similar physical properties to C2H4. It makes the step and the cost of C2H4 purification complex and expensive, so research of efficient C2H4 purification method is required for the sustainable development.We developed two aminal-linked covalent organic frameworks (COFs) for one-step C2H4 purification by selective C2H6 trapping. Their ethane-selective adsorption behavior, chemical and physical properties were confirmed by C2 gas isotherm, 13C solid state NMR, PXRD, etc. Detailed synthetic scheme and specific properties will be presented in the poster.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-97**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Exploration of electrochemical performance of Mn-substituted Li_2ZrCl_6 solid electrolyte for all solid state lithium batteries

Han Jin Jeon, Kwang Sun Ryu*

Department of Chemistry, University of Ulsan, Korea

Solid electrolytes are the key materials for next-generation lithium-ion batteries, offering significant advantages in terms of safety and energy density. Halide-based solid electrolytes, while exhibiting superior electrochemical stability compared to other solid electrolytes, face challenges in practical battery applications due to their low ion conductivity. In this study, in order to improve the low ionic conductivity, a strategy to increase the ionic conductivity by changing the Li^+ concentration and metal charge by doping Mn^{2+} in the trigonal Li_2ZrCl_6 is presented. Mn doped Li_2ZrCl_6 was synthesized through high-energy ball-milling. Structural analysis was conducted with powder X-ray diffraction, ^{7}Li-NMR, laser-raman, and X-ray Photoelectron spectroscopy. Electrochemical performance was evaluated through electrochemical impedance spectroscopy, cyclic voltammetry, and galvanostatic charge-discharge measurement. Each value of ionic conductivity in the bare and optimized compositions was 0.4 mS/cm and 0.8 mS/cm, respectively. Activation energy of Li_2ZrCl_6 and 5 mol% Mn doped Li_2ZrCl_6 is 0.342 and 0.326 eV. There is no electrochemical window difference between Li_2ZrCl_6 and 5 mol% Mn doped Li_2ZrCl_6. Galvanostatic charge-discharge was conducted to confirm cycling performance. The initial discharge capacities for Li_2ZrCl_6 and 5 mol% Mn doped Li_2ZrCl_6 are 185.6 and 171.6 mAh/g, respectively.

Poster Presentation : **INOR.P-98**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

High proton conduction through functional group modifications of porous organic polymers

Donggyu Lee, Chang Seop Hong[1,*]

chemistry, Korea University, Korea

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

Proton exchange membrane fuel cells (PEMFCs) have considered as an eco-friendly alternative energy production methods because hydrogen is used as fuel, thereby producing water only as a by-product. Recently, porous organic polymers (POPs) have been investigated as electrolyte of fuel cells due to its high stability and high conductivity in terms of long-term operation. Herein, a series of POPs were prepared through polymerization with phloroglucinol and aldehyde-containing monomer having different functional groups. To enhance conductivity, acidic groups were introduced to the POPs via sulfonation. The degree of sulfonation was controlled by functional groups from aldehyde-containing monomer. Hence, sulfonated POPs showed high proton conductivity. Detailed synthetic methods and characterization will be presented in the poster.

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Impairment of Bone Marrow Mesenchymal Stem Cell Differentiation by Tobacco Nitrosamines, Alleviated by Nanostructures

Nomundelger Gankhuyag, Jin Seok Lee[1,*]

Hanyang University, Korea

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

Smoking cigarettes is an alarming concern due to its strong association with tobacco-related cancers, often resulting in fatal outcomes. Tobacco comprises thousands of chemicals, with sixty-nine compounds identified as human carcinogens. Notably, among the tobacco-specific nitrosamines, 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) stands out as the most potent carcinogen. Mesenchymal stem cells (MSCs) are versatile cells capable of differentiating into various cell types and exhibiting robust immunoregulatory capabilities. Unfortunately, their regenerative potential becomes compromised by tobacco carcinogens. The impact of NNK-induced oxidative stress on MSCs remains elusive. This study delves into the influence of NNK on reactive oxygen species (ROS) within hMSCs. Additionally, we assessed MSC growth and NNK-induced osteogenic differentiation over 14 and 21 days. Consequently, escalating concentrations of NNK were found to impair osteogenic differentiation capabilities. Moreover, we also examined this effect on a substrate of silica nanobeads (SiNBs) with various diameters.

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Study of ROS concentration of Keratinocyte cells on nano-diamond substrates with various densities

Minseon Park, Jin Seok Lee[1,*]

chemistry, Hanyang University, Korea

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

Recently, there has been a surge in interest in research that delays or slows skin aging. In particular, keratinocyte cells are attracting attention as the main constituent cells that make up the human epidermis. Against this background, we aim to evaluate whether nano-diamond (ND) substrates can be utilized to reduce the aging process by inhibiting reactive oxygen species (ROS) production of paclitaxel (PTX)-treated keratinocyte cells. PTX is known as a drug that promotes aging by increasing ROS production in cells. Nano-diamonds are used because they have properties that reduce ROS concentration in cells, and we want to use these properties to decrease the aging effect of keratinocyte cells.In this study, a keratinocyte cell culture experiment was conducted by manufacturing substrates with various densities of ND particles. FACS measurements were performed to evaluate ROS concentration in cells, and Western blot analysis was conducted to identify protein markers related to aging. This study explores the possibility of mitigating the aging effect of PTX treatment of keratinocyte cells by utilizing ND particles, providing new insights into the field of skin aging research. Controlling ROS concentration in cells by controlling the microscopic properties of ND is expected to open up important applications for future beauty and skin health care as well as skin aging research.

Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Improved Extraction of Exosomes from Bovine Milk through the Integration of Electrophoretic Oscillation-Enhanced Tangent Flow-Driven Ultrafiltration Procedure

Hansol Lee, Minji Ko, Yuna Kwon, Young rag Do*

Department of Chemistry, Kookmin University, Korea

Exosomes, a common type of extracellular vesicle (EV), have gained considerable attention due to their potential applications in various fields including diagnostics, therapy, and serving as carriers for medications and skincare products. One method of isolating exosomes that has garnered interest is the tangent flow-driven ultrafiltration (TF-DU) technique. This approach employs SiNx membrane nanofilters, which can be adjusted to match the size of the target material. This effectively separates exosomes from bovine milk without distorting their shape or requiring specialized user skills. However, when using this method alone, there are some challenges. The small nanopores in the filter can become clogged by larger EVs and the proteins present in bovine milk. Another issue is the formation of a cake-like layer, which makes it difficult to consistently separate a substantial quantity of exosomes over prolonged periods. To address these challenges, a recent study combined electrophoretic oscillation (EPO) with the TF-DU method. This innovation helps dislodge larger EVs or clumped proteins from the filter pores, leading to improved filtration efficiency. By incorporating EPO into TF-DU, the problem of nanopore blockage due to larger bio-substances in milk was successfully avoided for more than seven days. The isolated exosomes, obtained through the TF-DU method enhanced with EPO, were estimated using a nanoparticle tracking analysis (NTA) to have a size of 124 nm. This advance holds promise for refining the separation of exosomes from complex biological mixtures, offering potential benefits for various applications.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-102**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

$LiTaO_3$ mixing effects to suppress the side reactions between electrolyte and cathode in all-solid-state batteries

Kwang Sun Ryu*, Kyu Sik Kim[1]

Department of Chemistry, University of Ulsan, Korea
[1]University of Ulsan, Korea

Suppressing the side reactions at the solid electrolyte-electrode interface in all-solid-state battery (ASSB) are very important to improve battery performance. Coating an electrochemically stable material on the surface of cathode has been used to suppress the side reactions occurring at interface between solid electrolyte and cathode. However, for effective suppression, the thickness of the coating film must be thin and uniform. Usually, an expensive ethoxide series must be used as a starting material. In this study, $LiTaO_3$ coating material was simply mixed with the solid electrolyte to measure the effect of suppressing side reactions. To synthesize the solid electrolyte $Li_{5.3}PS_{4.3}Cl_{1.7}$ and the mixing material $LiTaO_3$, high-energy ball milling and wet milling methods were used, respectively. The structural characteristics of the prepared solid electrolytes were studied by powder X-ray diffraction. The $LiTaO_3$ mixed solid electrolyte based ASSB showed a high discharge capacity of 177.3 mAh/g in the initial cycle, whereas the bare solid electrolyte ($Li_{5.3}PS_{4.3}Cl_{1.7}$) based ASSB showed a discharge capacity of 159.1 mAh/g. To understand the side reactions, electrochemical impedance spectroscopy (EIS) analysis was performed after galvanostatic charge-discharge cycles. The EIS analysis confirmed that the side reaction between a solid electrolyte and a cathode has been effectively suppressed in $LiTaO_3$ mixed solid electrolyte based ASSBs.

Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and characterization of Zn(II) precursors for atomic layer deposition

Ji Min Seo, Heesun Kim, Yongmin Go[1], Taek-Mo Chung[2], Ji Yeon Ryu, Bo Keun Park[*]

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea

[1]Department of Chemistry, KRICT, Korea

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

Atomic layer deposition (ALD) is a promising deposition method that is being researched and utilized in a variety of fields, including semiconductors, displays, and solar cells. In particular, as electronic devices become smaller and more complex, their reliance on ALD technology increases. ALD precursors for forming metal thin films require good volatility and fast chemical adsorption and surface reactions. Zinc oxide is a potentially useful material with high temperature safety and high electrical and thermal conductivity. Typically, zinc precursors such as alkyl zinc, zinc acetate, zinc chloride, and methyl zinc isopropoxide are used for ALD deposition of ZnO thin films. However, conventional zinc precursors produce corrosive byproducts and require high substrate temperatures for deposition. In this work, we synthesized a new precursor using an amino ketone ligand to solve the above problems. The newly synthesized zinc complexes were characterized by NMR, FT-IR, elemental analysis.

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Characterization of Germanium(II) Complexes for Atomic Layer Deposition

Heesun Kim, Ji Min Seo, Yongmin Go[1], Taek-Mo Chung[2], Ji Yeon Ryu, Bo Keun Park[*]

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea

[1]*Department of Chemistry, KRICT, Korea*

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

Thin films are used in a variety of applications such as batteries, displays, and memory. Thin film deposition methods include physical vapor deposition, CVD or MOCVD, and ALD. In recent years, the ALD process has gained traction for depositing thin films with precision and uniformity. ALD is a very suitable deposition method for precise film thickness and uniform conformal deposition, which requires a precursor with high volatility and thermal stability. Thin films containing germanium have found applications in many fields such as solar cells and microconductors. Among them, GeO2 has received much attention due to its high thermal stability on Si or Ge substrates and low leakage current in an electroless field. Therefore, in this presentation, we synthesized Ge(II) complexes to enable ALD to form germanium oxide (GeOx) thin films. The synthesized germanium complexes possessed good thermal stability, high volatilit. The complexes were characterized by 1H NMR, 13C NMR, FT-IR, elemental analysis (EA) and thermogravimetric analysis (TGA).

Poster Presentation : **INOR.P-105**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis of various novel scandium precursors for ALD

Yongmin Go, Bo Keun Park[1,*], Taek-Mo Chung[2]

Department of Chemistry, KRICT, Korea

[1]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

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

Scandium oxide (Sc2O3) has a dielectric constant of ~14 and a band gap of 6.3eV with high conduction and valence band offsets. In general, Sc(thd)3 and Sc(Cp)3 are mainly used to form scandium oxide. However, there are problems such as volatility, thermal stability, and reactivity, so it is necessary to develop new precursors having better properties. Therefore, we synthesized novel Sc precursors by introducing bidentate ligands. The precursors were confirmed by 1H-NMR, 13C-NMR, FT-IR, Element analysis (EA). Thermal properties and volatility of the Sc precursors were investigated through thermogravimetric analysis (TGA) and sublimation. The Sc precursors have higher thermal stability and better volatility than Sc(thd)3 and Sc(Cp)3, and is expected to be useful to scandium oxide thin films deposition using atomic layer deposition.

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Oxidation of aniline derivatives by catalytic reactions in HKUST-1 with hydrolytic stability enhancement for water harvesting

Byongjune Kim, Nak Cheon Jeong[1,*]

Department of Physics & Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics & Chemistry, DGIST, Korea*

Metal-organic frameworks (MOFs) have considered as one of the most interesting porous materials because of its high specific surface area and tunable porous environment. However, MOFs are not utilized in the industrial fields yet because of its 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 is used to determine the reason of enhanced hydrolytic stability after the reaction with aniline derivates. Furthermore, the extremely increased hydrolytic stability can be used as water harvesting metal-organic framework.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Audible Sound-driven Chemical Patterns in a Square Dish

Mingyu Kim, Ilha Hwang*, Kimoon Kim*

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

Chemical patterns in solution are generated by diffusion of colored chemical species from chemical networks operating under nonequilibrium conditions. Although various chemical reactions are known to form such patterns, they produce different patterns each time because the diffusion cannot be controlled as intended. Recently, we reported that the chemical pattern created in a Petri dish can be easily regulated by controlling the diffusion according to the frequency and intensity of the audible sound waves applied.[1-5] In this study, we investigated the effect of the shape of the dish, another important factor that has an impact on the shape of these chemical patterns. For example, we have investigated the effect of the frequency of the audible sound in the patterns produced by the methylene blue oxidation reaction in a square dish. This study opens up new possibilities for the spatiotemporal regulation of chemical reactions in a diverse but controllable manner.

(1) Hwang, I. et al., *Nat. Chem.* 2020, *12*, 808.
(2) Lee, I. et al., *J. Chem. Educ.* 2022, *99*, 1539.
(3) Dhasaiyan, P. et al., *Nat. Commun.* 2022, *13*, 2372.
(4) Choi, S. et al., *Chem* 2022, *8*, 2192.
(5) Sen, S. et al., *Chem* 2023, *9*, 624.

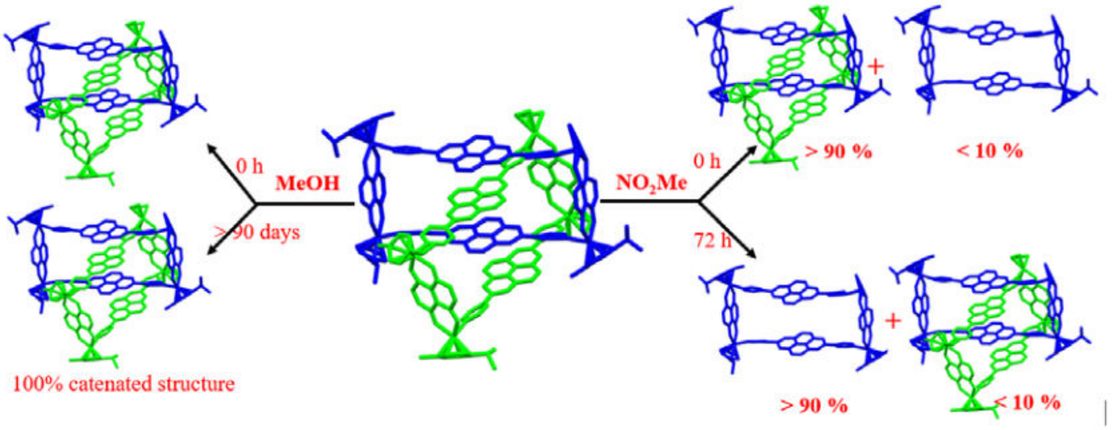
Poster Presentation : **INOR.P-108**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Pyrene-Functionalized Ru-Catenated Metallacycle: Conversion of Catenated System to Mono-Rectangle Through Aging

Chang Yeon Lee*, Woo Seong Jo, Gajendra Gupta

Department of Energy and Chemical Engineering, Incheon National University, Korea

Molecular transformation behavior within a mechanically interlocked system is often assisted by chemical manipulation such as inclusion of guest molecule, variation in solution concentration or swapping of solvents. Here we synthesized a ruthenium metal and large π-conjugated pyrene-based $(2+2)_2$ catenated rectangles which transforms into mono-rectangle in nitromethane at a constant concentration simply by standing or aging (Scheme 1). The catenated rectangles which is in majority at time 0 h interestingly transforms into mono-rectangle within 6 h in nitromethane, without any chemical manipulation, as confirmed by nuclear magnetic resonance spectroscopy. However, in methanol under similar condition it remains catenated for months and is the most thermodynamically stable species. Furthermore, theoretical calculations were studied to provide insights into the formation of catenated structure over other potential ring-in-ring or Borromean ring type structures. GFN2-xTB hatree calculation showed that the lower binding energy within the rectangles favors catenated structure over other potential ring-in-ring or Borromean ring type structures. This work represents a new example of intertwined structure which self-assembles into catenated ring rather than ring-in-ring or Borromean ring and transforms into mono-rectangle in nitromethane without the use of any template, alteration in solution concentration or exchange of solvents, but simply by standing at room temperature.



Scheme 1: Transformation behavior of pyrene-based catenated ruthenium metalla-rectangles to mono-rectangle in methanol and nitromethane.

Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Polyaniline-incorporated Metal-Organic Frameworks for Enhanced Hydrolytic Stability and Atmospheric Water Harvesting

Sun Ho Park, Nak Cheon Jeong[1,*]

Department of Physics & Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics & Chemistry, DGIST, Korea*

Adsorption-based atmospheric water harvesting (AWH) is attracting attention as a potential solution to address the global water scarcity crisis. Within this context, metal-organic frameworks (MOFs), a category of porous materials characterized by their high surface area and modifiable structures, have gained significant prominence as adsorbents for AWH applications. Although MOFs possessing open metal sites (OMS) show advantageous rapid water adsorption properties, their use in AWH has been limited due to their inherent challenges, including hydrolytic instability and energy-demanding water desorption. In this study, we report a novel approach involving the integration of polyaniline into HKUST-1, a prototypical MOF featuring OMS. This integration results in the formation of a composite material denoted as polyaniline-incorporated HKUST-1 (pAni-HK), which exhibits a substantial enhancement in hydrolytic stability. Remarkably, pAni-HK showcases swift adsorption kinetics at lower relative humidity (RH) levels, primarily attributed to its OMS, while its hydrophobic polyaniline component contributes to rapid desorption kinetics.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Characterization of Nickel(II) Complexes Supported by a Phosphine-Based Ligand

Yunjeong Park, Sol Bi Kim, Hyeonju Kim, Jin Kim[1,*]

Department of Chemistry, Suncheon National University, Korea

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

Due to their robustness and ability to accommodate a wide range of local geometries, pincer complexes can be utilized for a number of chemical transformations including coupling, bond cleavage, small molecule activation, etc. To investigate various activation reactions of small molecules, such as carbon monoxide, carbon dioxide, and sulfur dioxide, an air-stable complex (PPP)NiCl$_2$ [PPP = bis(2-diphenylphosphinoethyl)phenylphosphine] was prepared as precursor. To enhance the reactivity of the nickel center, the chloride anions were further substituted with non-coordinating anions. The syntheses of these nickel complexes along with their characterizations by various spectroscopic techniques and X-ray crystallography will be discussed.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Surface-Modified Zinc-Glutarate for Efficient Copolymerization of CO2 and Epoxides

Jong Doo Lee, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Due to the climate disaster by causing global warming, the catalytic conversion of CO2 into valuable chemicals is gaining attention as a strategy for reducing CO2 emissions. Zinc glutarate (ZnGA) is a catalyst for polycarbonates synthesis from CO2 and epoxides, but the low catalytic activity and CO2 fraction acts as a barrier of industrial application. Herein, we develop a surface modified ZnGA that have high surface area and microporosity (< 2 nm) by using special additives resulting high catalytic performances. By using acetic acid for reaction between ZnO and glutaric acid, thin plate morphology 2D-ZnGA was synthesized resulting more exposed Zinc atom that can activated from H3Co(CN)6 (Co-ZnGA). The Co-ZnGA have large surface area and pore volume (215 m2 g−1 and 0.28 cm3 g−1) that make effective access and interaction between epoxides and CO2. The synthesized Co-ZnGA catalysts exhibit highly improved copolymerization performance between CO2 and propylene oxide (855 g g-cat−1, fCO2=0.61), 1,2-epoxyhexane (1540 g g-cat−1, fCO2=0.91), 1,2-epoxybutane (1190 g g-cat−1, fCO2=0.83), and styrene oxide (148 g g-cat−1, fCO2>0.99). This study provides a new strategy using Co-ZnGA instead of conventional ZnGA for efficient copolymerization of CO2 and epoxides.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

High Selectivity of Alkenes Even with Extended Reaction Times for Semi-hydrogenation of Alkynes Using Pd4S nanoparticles on Sulfur-rich Hollow Carbons

Yoon Kee Kim, **Seung Uk Son***

Department of Chemistry, Sungkyunkwan University, Korea

Selective hydrogenation of alkynes to alkenes is pivotal for synthesizing various chemicals. However, obtaining specific alkene products instead of alkanes via semi-hydrogenation poses a significant challenge due to the risk of consecutive hydrogenation steps yielding unwanted alkanes. Concurrently, metal nanoparticles have gained attention as catalysts, despite their susceptibility to surface-related instability leading to aggregation and reduced activity.In response, counteractive strategies are emerging, with a primary focus on dispersing metal nanoparticles onto stable solid supports. Yet, these supports play a dual role – not only as physical foundations but also as regulators of catalytic behavior. This dual nature is notably pronounced in the context of strong metal-support interactions (SMSI), a pivotal factor in heterogeneous catalysis involving metals. Furthermore, solid supports can alter the electronic surroundings of metal nanoparticles, a phenomenon termed electronic metal-support interaction (EMSI).In this research, we successfully fabricate the H-SC@Pd4S catalyst, encapsulating Palladium within hollow-microporous organic polymers (H-MOPs) and incorporating sulfur. This strategic infusion of sulfur into the solid support enables the creation of catalysts that maintain high selectivity for alkene generation even during extended reaction durations. Additionally, the resultant catalyst showcases exceptional recyclability, upholding its efficiency over five cycles without succumbing to aggregation issues. This study not only advances the comprehension of catalyst design but also presents a pragmatic resolution to the intricate challenge of attaining pronounced selectivity in alkene production through the semi-hydrogenation of alkynes.

Poster Presentation : **INOR.P-113**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Synthesis of Microporous Organic Polymers with Tri-Zinc Macrocycles as Heterogeneous Catalysts for Converting Furan Esters Derived from Biomass into Polymer Precursors

June Young Jang, **Seung Uk Son**[1,*]

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

Petroleum-based plastics have been identified as a significant contributor to environmental issues due to their challenging post-use degradation. As a result, there is a thriving effort to replace conventional petroleum-based plastics with bioplastics or biodegradable plastics derived from plant-based biomaterials, aiming for easy post-use decomposition. To synthesize such biodegradable polymers, the creation of various environmentally friendly precursors is imperative. In this study, we have synthesized and utilized Microporous Organic Polymers (MOPs) with high surface area and remarkable chemical stability. These MOPs were synthesized using two building blocks: a tri-zinc macrocyclic compound and tetra(4-ethynylphenyl)methane, through the Sonogashira-Hagihara coupling method. The synthesized MOPs were utilized as heterogeneous catalysts with Lewis acidic properties. These MOPs exhibited a high surface area of 627 m²/g and demonstrated a uniform size of approximately 245 nm. In catalytic applications, diverse forms of furan-based diol precursors were synthesized for polyurethane synthesis from Dimethyl Furan-2,5-dicarboxylate (DMFDCA) through transesterification reactions with various diol. High yields of 99% were achieved within 9 hours, and successful reuse for up to 5 cycles was demonstrated. Moreover, one of the synthesized furan-based diol precursors was reacted with 1,6-Diisocyanatohexane to synthesize polyurethane, exhibiting a molecular weight of 43,000 (Mw), a Polydispersity Index (PDI) of 2.1, a thermal decomposition temperature (Td) of 298°C, and a glass transition temperature (Tg) of 6.7°C.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

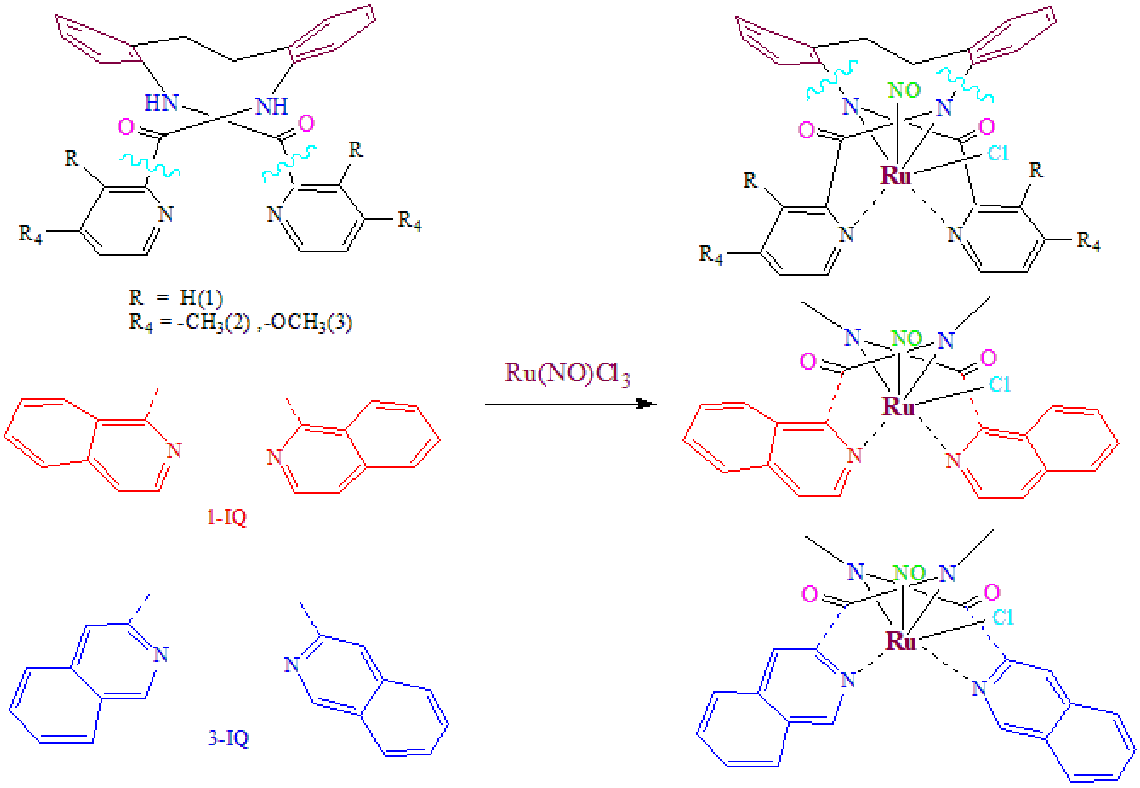
Exhibition Hall C THU 11:00~13:00

Photoactivated Release of Nitric Oxide from $\{\mathrm{Ru\text{-}NO}\}^6$ Complexes

Dae-Yeong Kim, Hong In Lee[1,*], Manho Lim[2], Seongchul Park[2]

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

The photolability of NO-containing transition metal complexes has recently been exploited in controlled delivery of NO. Among metal nitrosyls, ruthenium nitrosyls are a promising class of NO donor because of their increased thermal stability in biological media compared to other metal (Mn and Fe) nitrosyls. However, there is still a need to increase the efficiency (quantum yield) of NO release from ruthenium nitrosyls when exposed to lower energy light for delivery of NO to biological targets. Previously, we have reported the photoreactivity of [Ru(III)(epbp)(NO)Cl] where $\mathrm{epbpH_2}$ = N,N′-(ethane-1,2-diyldi-o-phenylene)-bis(pyridine-2- carboxamide). In the present study, we developed a series of [Ru(III)(R-epbp)(NO)Cl], (R=H, 4-$\mathrm{CH_3}$, 4-$\mathrm{OCH_3}$) and [Ru(III)(n-IQ)(NO)Cl], (n-IQ = 1,3-isoquinoline) complexes to observe the effects of the ligand frames on the photoreactivity of the complexes. To further improve the photoreactivity of the ruthenium complexes, we adopted dye chromophores to these nitrosyls and investigated their effects on the NO photolability.


HN
NH
O
O
R
R
R₄
R₄
N
N
R = H(1)
R₄ = -CH₃(2) ,-OCH₃(3)
1-IQ
3-IQ
Ru(NO)Cl₃
NO
Ru
Cl

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Mechanistic Study of Bis(dithiolene) W-oxo Complex: Identifying Proton Transfer and Potential-Directed Pathways

Wonjung Lee, Jaeheon Lee, Junhyeok Seo*

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

Dithiolene species have been found in molybdenum- and tungsten-containing oxotransferase and hydroxylase enzymes, as well as in formate dehydrogenase (FDH) and formylmethanofuran dehydrogenase (FMDH), used for converting of carbon dioxide to acetate or methane in organisms. These enzymes facilitate multiple proton/electron transfers and proceed catalytic reactions with high efficiencies. Inspired by these enzymes, several groups have reported the coordination of dithiolene ligands to transition metals such as Co, Ni, and Fe. Due to their easy one-electron transfer and unique electronic structure, low-valent metal complexes with bis(dithiolene) ligands exhibit unusual ligand-based interactions and numerous mechanistic and kinetic studies were reported. Recently, electrochemical exploration using high-valent W complex with dithiolene ligands has been undertaken, which proposed a catalytic reaction mechanism involving intramolecular hydrogen evolution between W-OH and W-hydride in W(lV)(OH)(H) intermediate using DFT calculation.Herein, we investigated the electrochemical behaviors of Bis(ditholene) W-oxo complex with several proton sources and examined the W-oxo intermediates. As a result, we could observe a unique anodic shift after the electrochemical reaction and determine a new reaction pathway of proton reduction. In this poster, we will discuss the current understanding of the Bis(ditholene) W-oxo complex and propose a new catalytic pathway for proton reduction using DFT calculation.

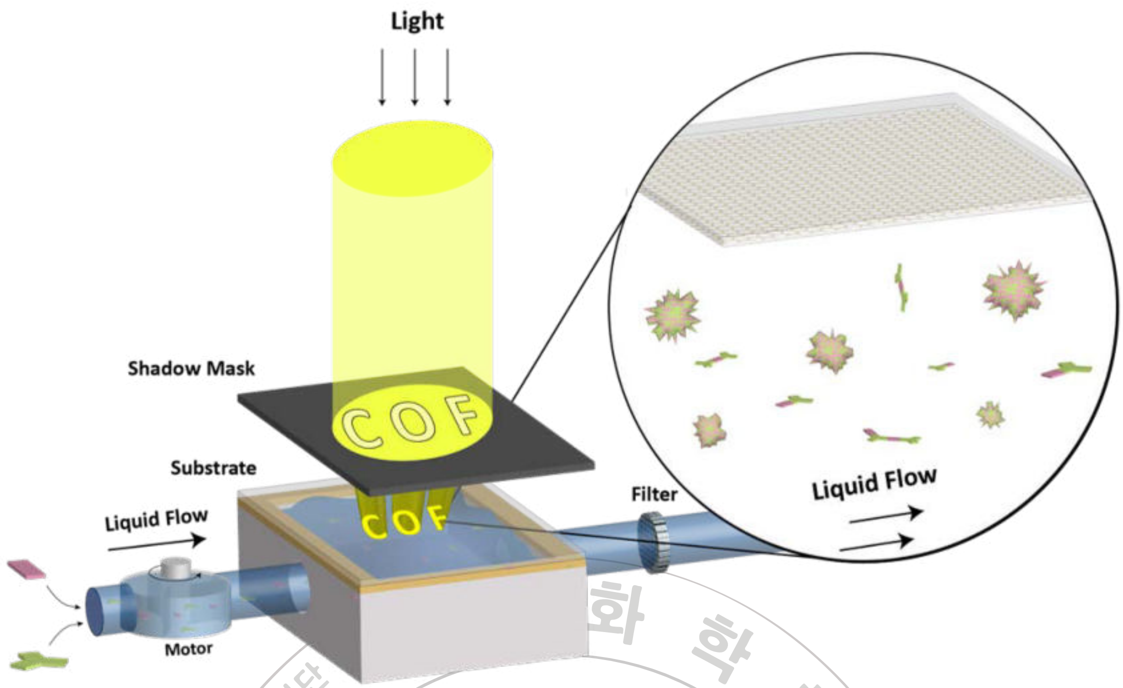
Poster Presentation : **INOR.P-116**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Photochemical and Patternable Synthesis of 2D Covalent Organic Framework Thin Film at Solid and Flowing-Liquid Interface

Hyunseob Lim*, Taewoong Kim

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

Two-dimensional covalent organic frameworks (2D COFs) are an emerging class of crystalline porous materials whose modular 2D structures and exceptional porosity has emerged as the appropriate candidate for a wide range of applications such as organic field effect transistors and optoelectronic devices. These applications require forming the material as a thin film, which has been achieved previously by enhancing the reactivity between organic building blocks selectively at the solid surface (on-surface synthesis) or liquid/liquid, liquid/gas interface (interfacial synthesis). This approach suffers from two key drawbacks: contamination from adsorbate of 2D COF powder or unreacted chemical species formed in liquid phase during on-surface synthesis and physical damage to the film in post transfer process during interfacial synthesis. Here we suggest the unique strategy for synthesizing homogeneous 2D COF thin film by combining photochemistry and liquid-flowing system. Liquid-flowing system could prevent the contamination due to the adsorbate and with photochemical approach the reaction-driving energy source can be introduced to the target substrate in the spatially controllable manner, which even facilitates the patternable synthesis of 2D COF. Owing to these merits, ultrasmooth patterned 2D COF film on 2D hexagonal boron nitride with highly ordered crystallographic orientation have been successfully synthesized. Our method enables the fabrication of optoelectronic device without pre- or post-processing, which will be used as the promising way for synthesizing high-quality patterned 2D COF films for various application fields.


Light
Shadow Mask
COF
Substrate
COF
Liquid Flow
Filter
Motor
Liquid Flow

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

The Effect of Diverse Anions in Heterometallic Au(I)-Ag(I) complexes

Jiyeong Song, Young-A Lee[*]

Department of Chemistry, Jeonbuk National University, Korea

A series of new heterometallic Au(I)-Ag(I) complexes, [AuAg(Spy)(PPh$_2$py)]X (X^- = $CF_3CO_2^-$, $CF_3SO_3^-$, SbF_6^-, NO_3^-, BF_4^-, PF_6^-, ClO_4^-), have been synthesized, and their physical properties have been studied. A series of new Au(I)-Ag(I) complexes was characterized by infrared spectra, ^{1}H NMR spectra, and single-crystal X-ray diffraction. The infrared spectra indicate the characteristic bands of the anion and the skeletal structure. There are three different types of structures depending on the anions. The complexes exhibit various inter- and intra- Au(I)-Au(I), Au(I)-Ag(I), and Ag(I)-Ag(I) interactions. The complexes with X^- = $CF_3CO_2^-$, $CF_3SO_3^-$, SbF_6^-, and ClO_4^- form dimers with intra Au-Ag and Ag-Ag interactions. In particular, the $CF_3CO_2^-$ anion coordinates with the Ag ion. Complexes with X^- = BF_4^- and PF_6^- are polymers that exhibit aurophilic interactions and do not have anion coordination. The polymeric complex with NO_3^- exhibits both aurophilic interactions and coordination with anions. The structures of these complexes are unlikely to be affected by only anion coordination ability. All of these complexes exhibit fluorescent properties and are planned to be studied for their potential applications in OLED display technology as dopant emitters, in solar photoconversion chemistry as chromophores, and in sensor development for luminescence detection.

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Wet-Chemical Synthesis of Diverse-Faceted Tungsten Oxide Photoanodes for Photoelectrochemical Water Splitting

Thandapani Marimuthu, Junhyeok Seo[1,*]

Chemistry, Gwangju Institute of Science and Technology, India

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

The manipulation of properties in the WO_3 photoanode through changes in facets plays a crucial role in enhancing both the kinetic and thermodynamic aspects of photoelectrochemical water splitting. In this study, we fabricated WO_3 photoanodes with different preferential growth facets: m-WO_3, 002-WO_3, and 202-WO_3, using a two-step chemical technique. The resulting WO_3 photoanodes exhibited monoclinic structures with wall-like morphologies composed of nanoparticles. The presence of W^{6+} and O^{2-} oxidation state in all photoanodes confirmed the formation of WO_3. Among these fabricated photoanodes, the 202-WO_3 photoanode exhibited better light absorbance with an energy band gap of 2.81 eV and a higher valence band maximum edge of 2.64 V relative to the water oxidation potential. Notably, the WO_3 photoanode with 202 facets demonstrated higher photoelectrochemical efficiency, characterized by a lower flat band potential of 0.57 V in comparison to other facets (002-WO_3) and (m-WO_3). Additionally, the WO_3 photoanode fabricated with 202 facets exhibited reduced charge transfer resistance (R_{ct}) at the interface between the photoelectrode and electrolyte when compared with other facets (002-WO_3 and m-WO_3). This finding indicates its potential for more efficient photoelectrochemical performance.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-119**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Overcoming phase purity, grains and surface defects challenges in copper bismuth oxide thin film photocathodes

Sakthivel Perumal, Junhyeok Seo[1,*]

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

The ternary spinel oxide, copper bismuth oxide (CBO) has attracted promising, earth-abundant semiconducting photocathode for photoelectrochemical (PEC) water splitting, if the issues of excessive charge carrier recombination and material degradation can be resolved, which are influenced by the bulk and surface quality. Phase-pure CBO films with good crystal quality need to be synthesized and investigated to address these problems and comprehend the underlying characteristics. But, it is challenging due to the spontaneous occurrence of copper and bismuth related impurity phases and significant defects such as copper or oxygen vacancies and grains. Reported here is an approach to overcome the phase-purity, grains and defects controlling challenges in complex CBO via simple solution process. Defects-less CBO films with larger crystalline grains are synthesized after studying the relationship between the crystal-structures, synthesis conditions, RTP, and properties over a range of thicknesses. Decreasing the Cu^{+1} /Cu^{+2} ratio of the CBO films reduces the amount of associated oxygen vacancies that increase the carrier (hole) concentration and greater the Fermi level, as evidenced by a shift in the flat band toward oxidation potentials. The optimum CBO film with enhanced light absorption and a shortened carrier diffusion pathway exhibited a high photocurrent density of 1.1 mA cm^{-2} at 0.4 V vs. RHE. This enhancement is related to reduced surface recombination, improved carrier extraction efficiency by enlarged grain size, improved the crystallinity and passivated the surface defect states.

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Exploiting dynamic bonding to activate open metal sites in HKUST-1 under mild conditions

Mariana Diaz Ramirez, Nak Cheon Jeong[1,*]

Physics and Chemsitry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics & Chemistry, DGIST, Korea*

Dynamic bonding in metal-organic frameworks (MOFs), the rapid dissociation and reassociation of metal-ligand bonds, has successfully explained some unexpected behaviors, such as the ability to undergo post-synthetic exchange or catalytic activity by saturated metal centers. Although most of the research interest has been focused on the metal–linker interaction, less attention has been paid to the interaction between solvent molecules coordinated with the metal centers that can be dissociated to yield open metal sites (OMS). Here, we hypothesize that coordinated solvent molecules also exhibit dynamic bonding between them and copper centers in HKUST-1 and that coordinated solvent molecules could be removed with a dry inert gas flow while transiently in the dissociated state. Moreover, the ease of dissociation of coordinated solvent molecules would depend on the bonding strength between the coordinated molecule and copper. A detailed investigation of the dissociation of solvents with increasing coordinating strength from Cu centers in HKUST-1 was carried out. Our findings revealed that weakly coordinating solvents like TCM and DCM dissociated at room temperature under the flow of dry inert gas. In contrast, more strongly coordinating solvents required higher temperatures for dissociation, however, we observed that full dissociation could be achieved at lower temperatures than conventional activation treatments. This work provides an effective method for OMS activation in HKUST-1 under mild temperatures and without hazardous chemicals.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis of Mono- and Divalent Copper Iodide Complexes with Bisquinoline Ligands

Eun su Chae, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Photoluminescent properties of metal complexes can be applied for LEDs or solar cells. Copper iodides, showing various structures and optical characteristics, are well-known for their photoluminescent properties.In this study, we synthesized two bisquinoline Schiff-base ligands to develop monovalent copper iodide complexes. Further, we reduced the ligands to ammines for being used to synthesize divalent copper iodide complexes. The monovalent copper complexes were structurally characterized to be coordination polymers with Cu_2I_2 cores. We discuss the photoluminescent properties based on the structural features of the monovalent complexes.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Electrocatalytic H_2 Evolution Reaction using Molybdenum Bis(dithiolene) complex with Cation

Yujin Baek, Junhyeok Seo[1,*]

Chemistry, Gwangju Institute of Science and Technology, Korea

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

Dithiolene complexes with transition metals were reported as electrochemical catalysts for hydrogen evolution reaction (HER). Dithiolene ligand participates in the redox process as it increases the electronic density and the overall basicity of the complex, thereby facilitating proton reduction. Dithiolene complexes containing earth-abundant metals such as Fe, Co, and Ni are reported to undergo HER reactions with protonation on the sulfur side. On the other hand, molybdenum and tungsten metals coordinated with bis(dithiolene) ligand have additional chalcogenide ligand (O, S, Se) on the axial site which makes the metal high-valent and plays an essential role in catalytic activity. Herein, we focus on the reactivity of the catalytic active site, the molybdenum-oxo ligand, depending on the acidity of the proton source. In addition, we will discuss how cation interacts with our complexes. The effect of cation on lowering the onset potential will be discussed at high pKa conditions where hydrogen bonding interactions are formed.

Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Formation of a 1D Poly-Pseudo-Rotaxane with Sulfur-Bearing Pillar[5]arene: Threading by Ion-Triplet and Organic Guest Molecules

Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

Poly-pseudo-rotaxanes are important in the fields of supramolecular chemistry and nanochemistry because they are functional structures with potential applications including drug delivery, materials design, and nanotechnology. In this work, a flexible sulfur-bearing pillar[5]arene (L) was synthesized and their supramolecular coordination networks are reported. The reaction of L with mercury(II) bromide afforded a one-dimensional (1D) poly-pseudo-rotaxane. In this structure, the $HgBr_2$ not only links the di-armed L ligands via an infinite -L-Hg-L-Hg- arrangement but also threads into a pillar[5]arene cavity in an ion-triplet form, (Br^--Hg^{2+}-Br^-). Reaction of L with mercury(II) bromide in the presence of the 1,2-dicyanoethane (C2) guest afforded a 1D coordination polymer with a poly-pseudo-rotaxane structure which shows C2 guest instead of $HgBr_2$ ion-triplet form in the pillararene cavities.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Analysis of lipid phase separation in senescence cells by single lipid tracking

Jiseong Park, Daeha Seo*

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

The cellular plasma membrane is comprised of several lipid domains, each measuring roughly 200 nm, which exist in a state of dynamic equilibrium. The lipid membrane phase separation has the ability to modulate the behaviors of biomolecules and subsequent signaling events. Changes in the lipid composition and organization of lipid rafts have been seen in a range of physiological contexts, including cellular senescence. Nevertheless, visualizing this phenomenon with sufficient spatiotemporal clarity continues to pose a challenge. In this study, we provide a single molecule analysis called the lipid-MAP (lipid molecular motion analysis pipeline) for the purpose of visualizing lipid nanodomains. The pipeline encompasses three basic steps: tracking individual lipid molecules, conducting state analysis through the utilization of a hidden Markov model (HMM), and estimating attributes related to the lipid domains. In this study, we employ the lipid-MAP technique to examine the influence of lipid composition on the phenomenon of lipid phase separation in both supported lipid bilayers and living cells. The reduction of cholesterol, which is recognized as a crucial constituent of lipid rafts, resulted in an enlargement of domain size and a decrease in variations in fluidity. We conducted an investigation on the disruption of lipid rafts in human dermal fibroblast cells at various stages of cellular senescence. The senescent cells exhibited a distinct disparity in fluidity between the two phases, alongside an observed augmentation in domain size when compared to young cells. Given the involvement of lipid rafts in various cellular signaling processes, it is hypothesized that they may play a role in the morphological changes and shortened division cycles in aging cells.

Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Spatiotemporal Control of Bacterial Motility and Photo-decomposition of Cu_2O NPs for Effective Antibacterial

Yongdeok Ahn, Daeha Seo*

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

The worldwide community acknowledges antimicrobial resistance as a significant peril to public health. In contrast to prior assumptions, recent research has revealed that antibacterial agents based on metals at the nanoscale can exhibit susceptibility to resistance. While the precise mechanism remains obscure, it is indisputable that repeated exposure can lead to the development of resistance, mostly due to the restricted effectiveness of antibacterial activity. This study introduces two strategies for creating a highly concentrated Cu^{n+} environment with the aim of enhancing antibacterial efficacy. One strategy involves the utilization of Cu_2O nanoparticles to induce thermal convection, hence facilitating the concentration of bacteria. The second strategy involves the utilization of light as a means to disintegrate nanoparticles, thereby generating Cu^{n+} in a highly rapid and forceful manner within regions afflicted by bacterial infestation. This experimental method illustrates that incarcerated microorganisms can be effectively eradicated within a brief timeframe. In addition, we propose the optimal morphological characteristics for Cu_2O nanoparticles in order to maximize their effectiveness through the controlled manipulation of facet junctions.

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Ferroelectric nanoparticles on Proteins in Alternating electric field

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*

Physical stimulation has been widely used to investigate various biological phenomena related to life and diseases, and electric fields have shown promising results in manipulating cellular component. Tumor Treating Fields (TTFields), low-intensity alternating electric fields, have been successful in disrupting polar proteins like tubulin, leading to delayed cell growth and apoptosis. Recent studies suggest that introducing ferroelectric nanoparticles can enhance TTFields' efficacy, but the underlying mechanisms remain unclear. In this study, we focused on the underlying mechanism using tetragonal BaTiO3 (T-BTO) nanoparticles with good biocompatibility and high spontaneous polarization as a representative ferroelectric material. We synthesized surface-modified BaTiO3 nanoparticles (T-BTO@SiO2@BODIPY, Transferrin) and investigated their effects in combination with TTFields on cell behavior. Our results revealed that T-BTO@SiO2@BODIPY, Transferrin significantly reduced cell proliferation compared to TTFields alone. Super-resolution radial fluctuation (SRRF) microscopy revealed the disruption of microtubules under TTFields, which was enhanced in the presence of nanoparticles. Despite considering the possibility of reactive oxygen species (ROS) generation and steric hindrance, our results did not support these hypotheses. Ultimately, we demonstrated the correlation of spontaneous polarization with the observed phenomenon. In conclusion, our study provides insights into the enhancement mechanism of TTFields using ferroelectric nanoparticles and contribute to valuable implications for future nano-therapies and drug development.

Poster Presentation : **INOR.P-127**
Inorganic Chemistry
Exhibition Hall C THU 11:00~13:00

Cu(II)-based 2D Single and Interpenetrated Networks depending on Coordination Environments.

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 behaviour 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.

Poster Presentation : **INOR.P-128**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Zinc(II) Coordination Compounds for Chemical Sensors

HyunSeo Kim, **Haeri Lee**[1,*]

Hannam University, Korea

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

Zn(II) coordination polymers allow to detect a toxic chemical 4-nitrophenol by electrochemical signals. The electrochemical measurement is a highly sensitive method providing evidence for chemical reactions on the surface of electrode. Hereby, we designed and synthesized new coordination structures containing imidazolyl donor ligands and Zn(II). The presence of microcrystals on the working electrode enhanced the redox signals.

Poster Presentation : **INOR.P-129**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Observing the Exchange of Motor Proteins in Live Cells using a Fourier Transform-Based Plasmonic Dark-Field Microscope

Siwoo Jin, Daeha Seo[*]

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

Intracellular cargo distribution heavily relies on the microtubule-driven motor transport mechanism, where motor proteins orchestrate movements to ensure precise delivery of organelles and proteins. This process involves coordinated motor actions, dynamically navigating obstacles by swapping at microtubule intersections. However, relying on translational motion alone lacks insight into motor protein attachment and detachment. Here, we present an innovative real-time quantification platform called a Fourier Transform-Based plasmonic dark-field microscope (FT-pdf), enabling measurement of azimuthal and polar angles with an impressive accuracy of 5 degrees. Employing this technique, we investigate prolonged endosomal dynamics, unveiling rotation patterns during intracellular transport. We further manipulate motor protein numbers using inhibitors, proposing a model that elucidates their effective search strategy. These findings offer insights into how the programmed cell efficiently regulates coordinated motor proteins within complex cellular environments, thereby optimizing material transport.

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Kinetic investigation of organic reactions on the single molecule

Minsoo Park, Daeha Seo[1,*]

Department of physics and chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

The 2o-amine catalysis has become a field of central importance for various organic synthesis, yet the reversible process of iminium ion formation remains ambiguous. Determining the mechanisms of chemical reactions is a crucial fundamental endeavor. However, Conventional measurements such as UV-vis absorption spectroscopy, mass spectrometer and 1H-NMR can hardly analyze each step of the reaction mechanism and static heterogeneity of kinetics. A single-molecule experiment shows the information hidden in ensembled-averaged methods. Here, to monitor the chemical reaction of individual molecule in real time, we present a reliable method by using organic dyes on total internal reflection fluorescence microscopy (TIRF), which allows us to track the reaction process at single-molecule level due to changes of conjugation length (π-π) and quantum yield. Statistical analyses of single molecule trajectories reveal molecular reaction kinetics of elementary reactions. This technique reveals optical properties of each intermediate/transition state in time trajectories which are otherwise difficult to detect with ensemble-averaged measurements.

Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Exploring Novel Approaches for Detecting Harmful Substances and Treating Related Diseases

JuHee Jang, Daeha Seo*

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

Detecting harmful substances and treating diseases caused by them are essential tasks for human health. Current methods for evaluating harmful substances involve utilizing animal experiments, cell assays, and chemical analyses to assess the safety of substances individually or in combination. These approaches primarily focus on organism and cell-level toxicity. However, it's crucial to acknowledge that even when substances meet established standard, they can still induce functional abnormalities within cells, potentially leading to a range of diseases. Moreover, addressing diseases caused by external environmental factors requires diverse treatment methods. Research involving various biological materials is being conducted to minimize drug-induced cell toxicity and to effectively deliver drugs to target tissues. In this study, we employed various reporter systems, including GCaMP, to promptly detect harmful substances by analyzing cellular signal patterns using fluorescence microscopy. Interestingly, even among substances below recognized toxicity thresholds, some disrupted cell signaling. This simple and cost-effective approach allows for rapid toxicity assessment. Additionally, the surface-engineered biological materials we developed have the potential to effectively store drugs and deliver them to target tissues through surface engineering. This cellular signal transmission-based platform and disease-treating biological materials have the potential to contribute to the effective detection of latent harmful substances and the treatment of diseases caused by them.

Poster Presentation : **INOR.P-132**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Controlling Intramolecular Charge Transfer on Proton-Coupled Electron Transfer (PCET) : in Co-Imbpy Complexes

JuEun Lee, Junhyeok Seo*

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

In the electrochemical hydrogen evolution reaction, 2 protons and 2 electrons are required. The proton-coupled electron transfer (PCET) associated with the pattern in which they are involved can be modulated through changes in both external and internal methods. External methods involve adjusting proton transfer (PT) by manipulating the pK_a of the proton source, or controlling electron transfer (ET) by tuning the strength of the oxidant, as in a hydrogen oxidation reaction. Internal methods involve incorporating proton relaying moieties to assist in PT. As an alternative internal method, we intended to control PCET by inducing intramolecular charge transfer within a complex. To achieve this, we introduced 2,2'-Bipyridine to modify the coordination structure. Through this approach, we observed that the pathways occurring in the electrochemical hydrogen evolution reaction can be controlled to follow stepwise ET/PT or concerted proton-electron transfer (CPET). This poster will elucidate the process of modulating PCET by inducing distinct intramolecular transfers in Co-Imbpy complexes.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Construction of Supramolecular Complexes by Host-Guest Interactions with Crown Ether-Armed Pillar[5]arene

Seohyeon Yun, Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

Crown ether-type macrocyclic ligands often show high selectivity for metal ions and these features make such molecules attractive candidates for separation and chemical sensing applications. We proposed a pillar[5]arene derivative that employs a crown ether including sulfur donors to accommodate metal cation in the cavity. In addition, the use of organic guest molecules is expected to induce the formation of mechanically interlocked molecules such as pseudo[1]catenane and pseudorotaxane by the host-guest interactions. For this reason, the crown ether-armed pillar[5]arene derivative (L) was synthesized and its supramolecular complexes were structurally characterized. Host-guest complexations between L and organic guest molecules is in progress.

Poster Presentation : **INOR.P-134**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Coordination Polymers of Polypseudorotaxanes of A1/A2 Thioglycolate-Armed Pillar[5]arene

Huiju Kim, Eunji Lee[1,*]

Chemistry, Gangneung-Wonju National University, Korea

[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Pillar[5]arene derivative having sulfur donor and carbonyl group could be a good candidate as a platform for the construction of coordination polymers with intriguing coordination modes via coordination bonds and supramolecular interactions. In this work, A rationally designed thioglycolate-bearing pillar[5]arene derivative (L) which employs pillar[5]arene moiety to accommodate a linear guest molecule in the cavity (host-guest interaction) and the sulfur donors for the soft metal coordination were synthesized. The preparation and characterization of polypseudorotaxanes with the organic guest molecules were investigated both in solution and solid states.

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Metallosupramolecules of Pillar[5]-*bis*-azathiacrown: Host-Guest Molecular Recognition and Coordination Networks

Hankyeol Park, Eunji Lee[1,*]

Department of chemistry, Gangneung-Wonju National University, Korea

[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Soft metal complexes of pillar[5]-*bis*-azathiacrown with flexible crown ether and their host-guest recognition using organic guest molecules are reported. In the reaction of pillar[5]-*bis*-azathiacrown with dinitrile guests $[CN(CH_2)_nCN$ (n=2-6: abbreviated C2-C6), all organic guests exist inside the pillar[5]arene cavity by CH···O and CH···π interactions. The reaction of pillar[5]-*bis*-azathiacrown with $AgBF_4$ gave a disilver(I) complex in which two silver(I) ions exist in the crown rings. In addition, guest molecular recognition of disilver(I) complex was confirmed by SCXRD and ^1H NMR experiments.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **INOR.P-136**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

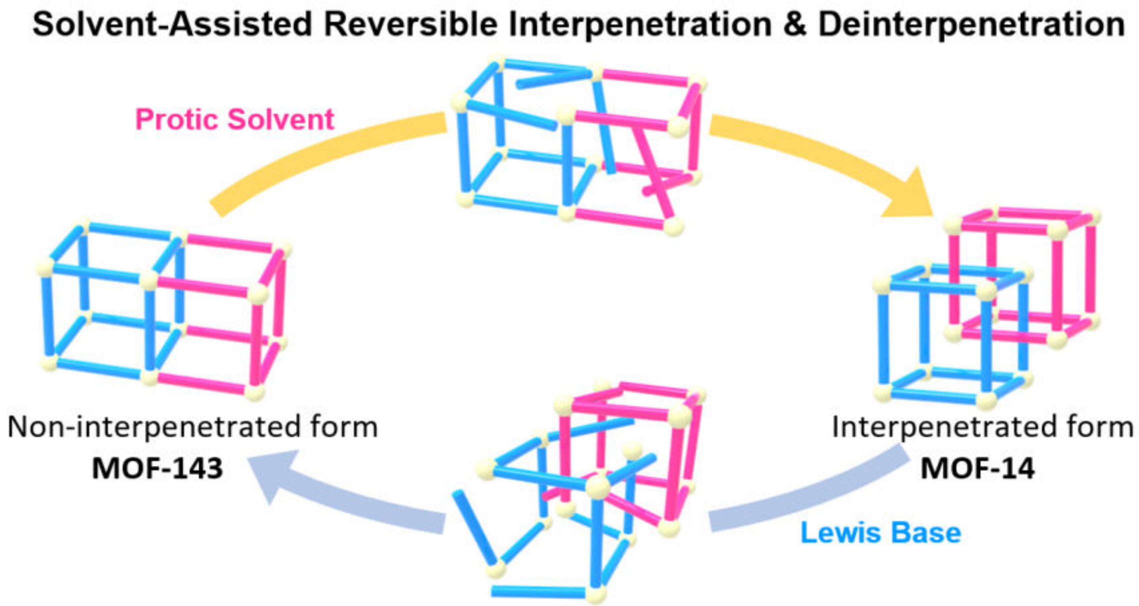
Solvent-Assisted Reversible Interpenetration of Cu(II)-Based Metal-Organic Frameworks: A Strategy for Enhancing Ethane and Ethylene Separation

<u>Cheol Yeong Heo</u>, Nak Cheon Jeong[1,*]

Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]Department of Physics & Chemistry, DGIST, Korea

Metal-organic frameworks (MOFs), a class of crystalline porous coordination polymers composed of metal ions and organic linkers, have been intensively studied for their ability to uptake non-polar 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 non-polar molecules due to their relatively higher stability and smaller micropores. This study reports the reversible interpenetration/de-interpenetration of MOF-143/MOF-14 through a solvent-assisted method. An initial water-activated phase of non-interpenetrated MOF-143 was converted into interpenetrated MOF-14 after treatment with small protic solvents and DMF. MOF-14 could also be converted into the non-interpenetrated form after a DMF and pyridine treatment. The reversibility of this interpenetration/de-interpenetration process was confirmed by sequentially converting MOF-14 into MOF-143. 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 non-interpenetrated 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.


Solvent-Assisted Reversible Interpenetration & Deinterpenetration
Protic Solvent
Non-interpenetrated form
MOF-143
Interpenetrated form
MOF-14
Lewis Base

Poster Presentation : **INOR.P-137**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Exploring NiS Nanoparticle-Embedded 3D Hollow Diatom Framework as a Unique Electrocatalyst for HER and DFT Analysis

Younghu Son, Bonseon Eo, GaEun Lee, Yunseul Kim, Minyoung Yoon[*]

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

For several years, embedding metal nanoparticles into porous materials has been widely conducted in various fields. However, the use of chemicals for synthesis of porous materials is toxic and expensive. Diatoms (Bacillariophyceae) are naturally available, having a typical three-dimensional (3D) porous hollow structure. We have developed a benign diatom/NiS hetero catalyst via the hydrothermal method. XPS, XANES, and EXAFS provided important information about the coordination with the diatom/NiS heterostructure. The diatom/NiS heterostructure catalyst exhibits excellent hydrogen evolution reaction (HER) activity, with an overpotential of -53.6 mV and Tafel slope of 55.1 mV dec^{-1} at a current density of -10 mA cm^{-2} in a 0.5 M H_2SO_4 medium. For the first time, we have analyzed the designed diatom/NIS catalyst activity using density functional theory (DFT) calculations based on the proposed diatom frame model. The theoretical results reveal that the intercalated NiS in diatom is an effective active site, and the calculated $\Delta GH*$ value for diatom/NiS is -0.05 eV. We also analyzed additional calculations to determine the activation energy barriers for Volmer and Heyrovsky reaction steps of HER employing the climbing-image nudged elastic band (CI-NEB) method. The NiS intercalated diatom (diatom/NiS) imparts a synergetic effect that accelerates the reaction kinetics on the catalytic active sites and decreases the charge-transfer resistance of the catalyst, leading to high HER activity and durability. Gas chromatography evaluated the produced H_2 gas, and the Faradaic efficiency was achieved at 99.74%. This developed benign catalyst serves as a next-generation eco-friendly electrocatalyst for energy harvesting.

Poster Presentation : **INOR.P-138**

Inorganic Chemistry

Exhibition Hall C THU 11:00~13:00

Detection of TNT Vapor Using Photonic Polymer Replicas Containing Silicon Quantum Dots with Distributed Bragg Structure

Jeong Kyeong Mun, Honglae Sohn*

Department of Chemistry, Chosun University, Korea

The fabrication of new functional materials tailored with novel physical and chemical properties represents one of the most crucial challenges in modern materials science. Nano-structured materials based on polymers composed with inorganic quantum dots are particularly attractive. Especially, the addition of semiconductor quantum dots to nano-structured polymer materials has led to markedly enhanced control of a wide range of technically important material properties from optoelectronic to mechanical properties. In this report, we describe a method for fabricating photonic polymer replicas containing silicon quantum dots. The photonic polymer replica with silicon quantum dots embedded in a polymer matrix exhibits both reflection and a photoluminescence property.This work was supported by the Technology Innovation Program (or Industrial Strategic technology development program, RS-2022-00154968)

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-139**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Temperature dependent ion aggregation behavior and spatial inhomogeneity in electrolyte solutions

Jonghyuk Ryu, Ravi Singh, Jiwon Seo, Jun-Ho Choi*

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

Some salts exhibit temperature-dependent solubility behavior in water. A notable example is potassium nitrate (KNO_3) with a solubility limit of 3.8 m at room temperature, showing a remarkable increase to 24.1 m at 100°C. On the other hand, NaCl shows a solubility limit of 6.2m at room temperature, with a slight increase to 6.7 m at 100°C. In the case of potassium thiocyanate (KSCN), the salt is highly soluble with a solubility of 22 m or more in all temperature ranges from 0 to 100 °C. In combination with graph theory and spatial inhomogeneity analyses from molecular dynamics trajectories in salt solutions, we investigate ion aggregation behavior and its impact on water H-bond structure at varying temperatures. It is observed that the three salts, NaCl, KSCN and KNO_3, undergo distinct temperature-dependent patterns and spatial distribution of ions in aqueous salt solutions. Furthermore, the differentiated aggregation pathway of ions is shown to affect the water structure and salt solubility in the binary mixtures.

Poster Presentation : **PHYS.P-140**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Photochemistry of thymine in solution revealed by an electrostatic embedding QM/MM combined with mixed-reference spin-flip TDDFT

Cheol Ho Choi[*], **Maryam Farmani**[1]

Department of Chemistry, Kyungpook National University, Korea

[1]*Chemistry, Kyungpook National University, Iran*

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 fittingfitted (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.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-141**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Changing Perspective: Upconversion Properties of Lanthanide doped NASICON

Young Gwon Jung, Kang Taek Lee*

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

As an alternative material for Li-ion batteries, the sodium superionic conductor (NASICON) got renewed attention due to their robust, high ionic conductivity, thermal-, air-, and water-stabilities. Meanwhile, in terms of structure, the NASICON has a highly disordered structure (non-centrosymmetric) which is preferred to the lanthanide upconversion (UC). UC is the phenomenon that generates higher energy photons by absorbing lower energy photons (e.g. NIR to VIS). This unique phenomenon involves forbidden 4f-4f transitions, thereby possessing low efficiency. However, according to the Judd-Ofelt theory, the non-centrosymmetric crystal interactions would partially allow the intra-4f transitions. This means the UC is much preferred in the disordered crystal systems, therefore, the fundamental studies for utilizing the NASICON-type crystal structure for UC are mandatory. Here, I synthesized the Er^{3+} doped $NaTi_2(PO_4)_3$ NASICON materials not as an all solid battery, but UC. We changed the perspective of NASICON as an alternative light emitting (optical) material.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-142**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

In-situ XPS study for Photocatalytic Performance Variations of ZnIn2S4 Nanoparticles Depending on Sulfur Source

Dung Hoang, Vy Pham[1], Hangil Lee[1,*]

Chemistry, Sookmyung Women's University, Korea

[1]Department of Chemistry, Sookmyung Women's University, Korea

ZnIn2S4 nanoparticle (NP) photocatalysts treated with different sulfur sources (thiourea (TU) or thioacetamide (TAA)) were successfully synthesized to investigate the wavelength-dependent photocatalytic activity owing to the concentration of Zn vacancies at the surface of the ZnIn2S4 NPs. in situ X-ray photoelectron spectroscopy were performed to investigate the effect of Zn vacancies on the photocatalytic activity of the ZnIn2S4–TU and ZnIn2S4–TAA NPs. Furthermore, the wavelength-dependent photocatalytic degradation (PCD) activity of the ZnIn2S4 NPs using 2,5-hydroxymethylfurfural (HMF) was investigated over a wide range. The selective oxidation of HMF using ZnIn2S4–TU NPs resulted in the formation of 2,5-furandicarboxylic acid via 2,5-diformylfuran with an efficiency of over 40% over a wide wavelength range. Thus, the irradiation wavelength for PCD depended on the number of defect structures introduced into the ZnIn2S4 NPs by the sulfur source.

Poster Presentation : **PHYS.P-143**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Solvent effects and pH dependence of the X-ray absorption spectra of proline from electrostatic embedding quantum mechanics/molecular mechanics and mixed-reference spin-flip time-dependent density-functional theory

Woojin Park, Cheol Ho Choi[1,*]

Chemistry, Kyungpook National University, Korea

[1]Department of Chemistry, Kyungpook National University, Korea

X-ray absorption spectroscopy (XAS) can provide element-specific local electronic information during chemical transformations when combined with quantum chemical simulations. In this contribution, we develop an efficient theoretical model for simulating the solvent effects on XAS, based on the combination of electrostatic embedding QM/MM and mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT). As a test case, we compute the C, N, and O K-edge X-ray absorption spectra of different protonation forms of proline. We show that the $1s \rightarrow \pi*$ transitions experience a small rigid shift with respect to the gas phase due to the canceling effect of the red shift due to structure fluctuations and the blue shift due to electrostatic interaction with water. The $1s \rightarrow \sigma*$ transitions, on the contrary, are more impacted by the fluctuation of proline structure and the electrostatic interaction with the solvent, which affects the mixing with Rydberg-type orbitals. By reconstructing the pH-dependent spectra, we determine that the N K-edge of proline can potentially be used to distinguish the cationic, anionic, and zwitterionic forms of proline.

Poster Presentation : **PHYS.P-144**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Understanding of Protein-Peptide Binding Using Artificial Intelligence and Large-Scale Molecular Dynamics

Se-Jun Kim, Da-Eun Hwang[1], 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-145**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Fluorescent Protein Charge in Protein Aggregation

Minchae Kang, Hyeryeong Lee[1], Sang Hak Lee[1,*]

Department of chemistry, Pusan National University, Korea

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

Protein aggregation is implicated in neurodegenerative disorders such as Alzheimer's Disease (AD), Parkinson's Disease (PD), and Amyotrophic Lateral Sclerosis (ALS). Our previous work demonstrated the essential role of small charged molecules in the formation of charged-protein aggregates. Furthermore, we identified that multivalently charged small molecules act as crucial bridges between charged proteins, facilitating aggregate formation. Since charged proteins create condensates by interacting with counterion, the charge of fluorescent protein is very critical in study protein phase separation or aggregation. In this study, considering the influence of protein charge, we investigated whether conjugated fluorescent proteins could impact aggregation. To explore this, we selected six fluorescent proteins; eGFP (-7.2e), mCherry (-5.4e), Dronpa-3 (-3.3e), mCyRFP1 (+0.5e), mEos3.2(+0.7e), and mPapaya1 (+3.3e). They are similar sizes but differing charges. Using TAR DNA binding protein 43 (TDP-43) and FUsed in Sarcoma (FUS) protein, we found that the protein aggregation (or phase separation) can be varied depending on the charge of fluorescent proteins.

Poster Presentation : **PHYS.P-146**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Quantum and Semi-classical Dynamics for a Simultaneously Coupled Bond-Breaking and Bond-Making in the Bi-directional Proton-Coupled Electron Transfer Process of FHCl

Pinit Ariyageadsakul, Kyoung-Koo Baeck[*]

Department of Chemistry, Gangneung-Wonju National University, Korea

We recently reported the nuclear wave-packet propagation dynamics of the bi-directional proton-coupled electron transfer (PCET) process starting from the charge-separated excited state of FHCl, F^+HCl^-. The study disclosed an interesting result that the dissociation through the PT channel (F + HCl) dominates over the ET (FH + Cl) channel in spite of the fact that the dissociation limit of the PT channel has higher energy than the limit of the ET channel. Simply stated, the movement of the heavier proton favors the movement of the lighter electron. To provide a more detailed insight on the very moment of its critical point of dynamics, as well as some complimentary classical insights in addition to quantum dynamical results, we carried out a semi-classical dynamics study using the SHARC (Surface-Hopping including ARbitary Couplings) program package with the MS(5)-CASPT2(17,11)/aug-cc-pVTZ level of ab initio theory. The statistical analyses for nuclear motion, population dynamics, and branching ratio were carried out with the ensemble of classical trajectories from 100 initial conditions. The changes of natural transition orbitals (NTOs) along representative classical trajectories were also analyzed to provide a better insight into the sub-femtosecond change of the net distribution of electronic charge. The results of the present semi-classical work and the previous full quantum dynamics study give more detailed insights into the critical situation governing the coupled situation of breaking and making chemical bonds in the bi-directional PCET process starting from the charge-separated state, F^+HCl^-.

Poster Presentation : **PHYS.P-147**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Predicting Electron Affinity of Polycyclic Aromatic Hydrocarbon Molecules

Jinmin Lee, Sang Hak Lee*

Department of Chemistry, Pusan National University, Korea

Polycyclic aromatic hydrocarbon (PAH) molecules are the building blocks of graphene. The electron affinity (EA) of PAH is a fundamental property to understand the electronic properties of graphene; however, it is difficult to directly observe EA using photoelectron spectroscopy. Thus, we tried to find the best theoretical method to predict the EA of PAH molecules. Therefore, we employed 13 different functionals: the five generalized gradient approximation (GGA) functionals, two meta GGA functionals, four hybrid GGA functionals, and two double hybrids GGA functionals. For already experimentally measured molecules, we performed theoretical (density functional theory) calculations using 13 different functionals to predict EA and compared the results with experimentally measured EA values. When compared to the difference from the experimental value, the two double hybrids GGA functionals, which required the longest time, showed an error of - 0.46 eV, and the five generalized gradient approximation (GGA) functionals, two meta GGA functionals, four hybrid GGA functionals showed errors of 0.24 eV, 0.10 eV, and 0.10 eV, respectively. Among GGA functionals, we found that three functions, BPW91, PBEPBE, and BPBE, provided accurate predictions when compared through mean absolute deviation (MAD), root mean square (RMS), and regression analysis.

Poster Presentation : **PHYS.P-148**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Elucidating Molecular Mechanism underlying the Alpha-Synuclein Aggregation or Phase separation

Kyubin Lee, Jinmin Lee[1], Sang Hak Lee[1,*]

Pusan National University, Korea

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

Parkinson's disease is a neurodegenerative disorder characterized by the abnormal aggregation of α-synuclein, which is implicated in its onset and progression. Given α-synuclein's overall negative charge, our hypothesis posited that charge-charge interactions between the protein and small charged biomolecules could drive aggregation. Notably, the folded segment of α-synuclein holds a partial positive charge, facilitating its anchoring to the cell membrane. Conversely, the exposed disordered region facing the cytosol bears a negative charge. Consequently, our study delved into α-synuclein aggregation and phase separation on lipid bilayers, investigating the influence of polyamine concentration and time. Our findings demonstrated that α-synuclein condensates formed notably at elevated polyamine concentrations. This underscores the pivotal role of positively charged biomolecules, specifically polyamines, in facilitating the aggregation or phase separation of negatively charged α-synuclein.

Poster Presentation : **PHYS.P-149**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Multi-reference Second-Order Perturbation Theory (MRPT2) with Adaptive Sampling Configuration Interaction Self-Consistent Field (ASCI-SCF)

Kyeong Su Min, Jae Woo Park[*]

Department of Chemistry, Chungbuk National University, Korea

In quantum chemical calculations, appropriate descriptions of electron correlation (static and dynamical) are necessary for obtaining accurate energies. One needs to include many electron configurations (Slater determinants) in the wave function to recover static correlation in highly correlated systems. A popular choice for this is complete active space (CAS), which is conceptually simple. Unfortunately, it is not possible to use large active spaces with CAS, as the number of configurations grows exponentially with respect to the number of active electrons and orbitals. The adaptive sampling configuration interaction (ASCI) method samples dominant determinants in the CASCI wave function. Because the ASCI self-consistent field (ASCI-SCF) method incorporates only correlation energies in the active space, one must also correct for the dynamical correlations.In this presentation, we present the second-order complete active space perturbation theory (CASPT2) an *N*-electron valence state perturbation theory (NEVPT2) with the ASCI self-consistent field (ASCI-SCF) reference function so that one can obtain a balanced description of static and dynamical correlations. We implement a direct method to calculate the intermediate matrices in CASPT2 and NEVPT2 to reduce the memory requirement for storing the four-particle reduced density matrix. We demonstrate our methods in computing the singlet-triplet gaps in several polyacene systems with active spaces up to (30*e*, 30*o*).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-150**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Highly Efficient T_1 MRI Contrast Enhancement using D-glucuronic acid coated mixed Zn(II)/Gd(III) oxide nanoparticles

Tirusew Tegafaw, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this work, we synthesized nanoparticles consisting of mixed Zn(II)/ Gd(III) oxides, with a molar ratio of approximately 8:92, and coated them with D-glucuronic acid. The average particle diameter (d_{avg}) was measured at 2.1 nm. The reduction in magnetization observed in the mixed nanoparticles is ascribed to the presence of non-magnetic Zn within the particle structure. These nanoparticles exhibited a longitudinal relaxivity (r_1) of 12.3 $s^{-1}mM^{-1}$ with r_2/r_1 = 1.1. We characterized particle diameter, hydrodynamic diameter, surface coating, magnetic properties, cellular cytotoxicity, water proton relaxivities, and in vivo T_1 MR Images. Highly positive contrast enhancements were observed in T_1 MR Images of a mouse.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-151**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

T_1-T_2 Dual-Modal MR Imaging: ultrasmall Gd_2O_3 coated by Polyaspartic Acid

Dejun Zhao, **Gang Ho Lee**[1,*]

Department of Chemistry, Kyungpook National University, China

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

Based on the well-known contribution of surface-coating of polymers on the nanoparticles for MRI, ultrasmall Gd_2O_3 nanoparticles were coated by Polyaspartic Acid with 2.0 nm average particle diameter, obtained through facile polyol method. The longitudinal (r_1) and transverse (r_2) of designed nanoparticles showed 19.1 and 53.7 $s^{-1}mM^{-1}$ at the 3.0 T MR field, respectively. Due to the appreciable r_2/r_1 ratio of 2.8, T_1 and T_2 MR images could be obtained, meaning that the designed sample has potential as dual-modal T_1-T_2 MRI contrast agent.

Poster Presentation : **PHYS.P-152**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Polyacrylic Acid-Coated Terbium(III) and Holmium(III) Oxide Nanoparticles: Synthesis, Characterizations, and 9.4 Tesla T_2 MR Imaging

Abdullah Al Saidi, Gang Ho Lee[1,*]

Chemistry, Kyungpook National University, Oman

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

Synthesized, characterized, and investigated as a new class of negative (T_2) magnetic resonance imaging (MRI) contrast agents at high MR fields are polyacrylic acid (PAA)-coated lanthanide oxide (Ln_2 O_2) nanoparticles (NPs) (Ln = Tb and Ho) with high colloidal stability and good biocompatibility. Their r_2 values were appreciable at a 3.0 T MR field and greater at a 9.4 T MR field, while their r_1 values were negligible at all MR fields, indicating their exclusive induction of T_2 relaxations and negligible induction of T_1 relaxations. Strong negative contrast enhancements in in vivo T_2 MR images at a 9.4 T MR field after intravenous administration into the tails of rodents confirmed their effectiveness as T_2 MRI contrast agents at high MR fields.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-153**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Glucosamine-Conjugated Polyacrylic Acid-Coated Ultrasamll Gadolinium oxide Nanoparticles as Tumor Targeting Positive Magnetic Resonance Imaging Contrast Agents

Ying Liu, Gang Ho Lee[1,*]

Department of Chemistry, Kyungpook National University, China
[1]Department of Chemistry, Kyungpook National University, Korea

Monodisperse and ultrasmall polyacrylic acid-coated gadolinium oxide nanoparticles (PAA-UGONs) (d_{avg} = 1.76 nm) were synthesized and the PAA-UGONs were conjugated with glucosamine (GlcN) by EDC/NHS method. The nanoparticle solution were stable and non-toxicity up to 0.5 M Gd. Their performance as a positive (T_1) magnetic resonance imaging contrast agent was investigated. The PAA-UGONs and GlcN-PAA-UGONs exhibited three to four times higher r1 values than those of commercial Gd-chelates, and their r_2/r_1 ratios were close to one. The higher positive (T_1) contrast enhancements at various organs including tumor site (in human brain glioma U87MG tumor-bearing mice) were observed, indicating that they can serve as T_1 MRI contrast agents. Compared with PAA-UGONs, the contrast enhancements of the GlcN-PAA-UGONs were the highest in the tumor site, owing to a higher demand for glucosamine in metabolic processes in tumors cells than in normal cells (i.e., GlcN effects). These results demonstrated that GlcN-PAA-UGONs are the potential excellent T_1 MRI contrast agents in tumor targeting imaging.

Poster Presentation : **PHYS.P-154**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Biotin-Conjugated Poly(Acrylic Acid)-Grafted Ultrasmall Gadolinium Oxide Nanoparticles for Enhanced Tumor Imaging

Mohammad Yaseen Ahmad, Gang Ho Lee[1,*]

Department of Chemistry, Kyungpook National University, India
[1]*Department of Chemistry, Kyungpook National University, Korea*

Herein, biotin (Bio)-conjugated poly(acrylic acid) (PAA)-grafted ultrasmall gadolinium oxide nanoparticles (Bio-PAA-Gd_2O_3 NPs) were synthesized for enhanced tumor imaging using Bio as a tumor-targeting ligand. The average particle diameter of Gd_2O_3 NPs was 2.1 nm. The Bio-PAA-Gd_2O_3 NPs exhibited excellent colloidal stability (i. e., no precipitation) and a high longitudinal water proton spin relaxivity (r_1) of 23.8 s^{-1} mM H^{-1} (r_2/r_1=1.6 and r_2=transverse water proton spin relaxivity), which was ～6 times higher than those of commercial Gd-chelated magnetic resonance imaging (MRI) contrast agents. Cytotoxicity tests using two cell lines showed that the Bio-PAA-Gd_2O_3 NPs were almost non-toxic up to the measured concentration of 500 μM Gd. The enhanced tumor imaging of the Bio-PAA-Gd_2O_3 NPs was demonstrated through their higher positive contrasts and longer contrast retention at the tumor after intravenous injection in T_1 MR images, compared with those of the control (PAA-Gd_2O_3 NPs).

Poster Presentation : **PHYS.P-155**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Aggregation and Disaggregation of FUS Protein

Hyeryeong Lee, Sang Hak Lee*

Department of Chemistry, Pusan National University, Korea

FUS (FUsed in Sarcoma) protein aggregation is the main cause of amyotrophic lateral sclerosis (ALS), one of the neurodegenerative diseases. It is known that the low complexity domain (LCD) of FUS is an intrinsically disordered domain and negatively charged (-4 e). On the other hand, the c-terminal domain (CTD) is positively charged (+18 e) at the physiological condition. Due to their strong charge, they are not able to be aggregated by themselves. Therefore, we thought that there might be a multivalent cation and anion to create the protein aggregation. Thus, we were interested in investigating small multivalent charged biomolecules, including polyamine and ATP molecules. We found that, when adding polyamine molecules to e-coli, the LCD-expressed cell showed aggregated proteins. In the case of CTD, we observed the CTD expressed showed protein aggregation in response to supplemented ATP in the media. We concluded that multivalent charged molecules, such as polyamine (cationic) and ATP (anionic), are mainly attributed to the FUS aggregation in cells. In addition, we also found that when we disrupted polyamine molecules in cells using NO gas which created NONOate after reaction with polyamine, protein aggregation did not observe anymore. This indicates that polyamine molecules play a critical role in protein aggregation and NO gas can be one of the solutions to prevent cells from creating protein aggregation.

Poster Presentation : **PHYS.P-156**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Regulation of cellular expression level of MMP-9 by vitamin A, B, C, and D

Min Jung Kim, Namdoo Kim[1,*]

Kongju National University, Korea

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

Matrix metalloproteases (MMPs) are a family of zinc-dependent endopeptidases that play important roles in a variety of pathological and physiological processes. Degradation of the extracellular matrix (EM) involved in tissue repair, development, and morphogenesis is a major function of MMPs. One of the MMPs, MMP-9, is induced by various inflammatory stimuli and degrades type IV collagen in the basement membrane to promote cancer cell movement. In this study, we focus on vitamins that might be potential inhibiters for MMP-9 expression. Mammalian cells were treated with different doses of water-soluble vitamins (B and C) and fat-soluble vitamins (A and D). 24 hours after transfection, cells were fixed and immunostaining was performed. Fluorescence images were taken and mean fluorescence intensities at different doses were compared with each other. As a result, fat-soluble vitamins significantly lowered the expression level of MMP-9, whereas water-soluble vitamins did not show such an effect.

Poster Presentation : **PHYS.P-157**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

A Study on the Effect of Vitamins on cellular expression level of MMP-2

Hyunlyong Lee, Namdoo Kim[1,*]

Department of Chemistry, Kongju National University, Korea

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

MMP-2 (Matrix metalloproteinase-2) is a member of the endopeptidase that contains zinc(II) for activity. Its important role is to degrade the extracellular matrix (EM) by type IV collagen degradation. Tumor cells usually have high levels of MMP-2, and this function promotes cancer progression and metastasis. In addition, many diseases such as Alzheimer's disease, Stroke, Cardiovascular diseases are related to the expression level and activity of MMP-2. Here, we investigated cellular expression level of MMP-2 according to the vitamin dose. Cells were treated with various doses of vitamin A, B, C and D, respectively after transfection. After immunostaining, fluorescence images were acquired to quantify the expression level. Is was observed that vitamin A and D lowered the expression level of MMP-2 while no significant changes were observed with vitamin B and C.

Poster Presentation : **PHYS.P-158**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Optical gain in colloidal quantum dot film under nanosecond optical pumping

Suhyeon Kim, Jiwon Bang*

Department of Chemistry, Incheon National University, Korea

Semiconductors with quantum confinement effects have garnered significant interest as promising gain media for lasers. Notably, colloidal quantum dots (CQDs) have captured considerable attention as versatile gain materials due to their ability to be processed in solutions with size-tunable optical transition. However, the strong Coulomb interactions in three-dimensional quantum confinement of CQDs utilized as gain media have posed challenges by substantially accelerating the rate of Auger non-radiative decay, which leads to very fast deactivation of optical gain. Consequently, to enable the practical realization of CQD lasers, operation under continuous pumping conditions is imperative. However, thus far, laser demonstrations of CQDs have primarily relied on ultrafast pulse excitation to preserve the population inversion state. Herein, we present the demonstration of amplified spontaneous emission (ASE), a prerequisite for achieving lasing action, in colloidal CdSe/CdS/ZnS QDs under nanosecond pulsed optical pumping. The thick CdS shell layer onto the CdSe core QDs results in the spreading of the electron wavefunction into the CdS shell layer. This spatial redistribution reduces the biexciton Auger rate to ~ 109 s-1. Furthermore, the outermost ZnS shell layer serves to protect the QDs under harsh pumping conditions as well as suppresses energy transfer between closely packed QDs within solid films. The closed-packed QD film exhibits amplified emission under 355 nm optical pumping with 6 ns pulse width. The characteristics of the ASE in the QDs are investigated through variations in pump power, film structure, and strip length. The proposed QD structure holds substantial promise as an attractive candidate for the development of practical applied QD laser systems.

Poster Presentation : **PHYS.P-159**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Selective Binding of SERS-Active Fe_3O_4@Au NPs@SiO_2 to Circulating Tumor Cells

Hae-jin Chung, Eungyeong Park, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

Circulating tumor cells (CTCs) have the ability to detach from the primary tumor and disseminate through the bloodstream, potentially leading to the development of new disease sites. In the concept of liquid biopsy, CTC detection emerges as a promising method for early tumor diagnosis. In this study, we used surface-enhanced Raman scattering (SERS) as an innovative technique known for its superior sensitivity, selectivity, and photostability, to provide a more accessible alternative to traditional biopsy methods.We focused on the fabrication of Fe_3O_4@Au nanoparticles@SiO_2 (Fe_3O_4@Au NPs@SiO_2) for SERS applications. By incorporating a magnetic Fe_3O_4 core, Fe_3O_4@Au NPs@SiO_2 can easily isolate cancer cells from complex biological systems.The properties of the Fe_3O_4@Au NPs@SiO_2 are thoroughly examined through comprehensive characterization, including transmission electron microscopy, UV-vis absorption spectroscopy, and SERS analysis.This study highlights the potential of these nanoparticles to transform early-stage diagnosis techniques, providing a more efficient and minimally invasive approach.

Poster Presentation : **PHYS.P-160**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Screening Cancer Cell Lines Using Deep-UV Resonance Raman Spectroscopy

Ah-hyun Woo, Sila Jin[1], Yeonju Park[2], Jongmin Park[3], Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea

[1]*Department of Chemistry, University at Albany, SUNY, USA,, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

[2]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

[3]*department of Chemistry, Kangwon National University, Korea*

Recent studies have highlighted the significance of utilizing exosomes for early cancer diagnosis and monitoring the effectiveness of anticancer therapies. Exosomes present in body fluids provide various cellular information, holding great promise for sensitive cancer diagnosis while minimizing patient suffering from biopsy. Raman spectroscopy is a powerful method for cancer diagnosis because it reveals material-specific information in the finger print region. However, it is difficult to obtain biological sample spectra with visible light lasers because most biological samples emit strong autofluorescence in the region above 260 nm. In this study, to overcome the autofluorescence of exosomes, deep-UV (244 nm) laser was used. Deep-UV Raman spectra of exosome extracted from various cell lines were obtained, and principal components analysis (PCA) analysis was performed. Details of analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-161**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Effect of Electromagnetic Field Effect on Charge Transfer in Semiconductor By SERS Activity of PS/Ag/MoO_3 Film

YoonSeop Byun, Shuang Guo, Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea

In this study, we fabricated a PS/Ag/MoO_3 film utilizing a layer-by-layer approach including sputtering deposition method. The film was constructed by sequentially depositing layers Ag and MoO_3 on a hexagonal close packing polystyrene substrate. Using 4-mercaptobenzoic acid (4-MBA) as probe molecules, surface-enhanced Raman scattering (SERS) spectra were used to study metal-semiconductor molecular interfaces. Our study mainly focuses on investigating the electromagnetic (EM) effect on the charge transfer (CT) in semiconductor with changes in film thickness. These thickness variations were achieved by adjusting the sputtering deposition time for Ag. The results of this study are expected to contribute to the research and development of semiconductor-based SERS substrates by elucidating the interplay of EM and CT effects. It has the potential to pave the way for customized applications in the field of SERS.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-162**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Effect of Ag-rGO Structure on the SERS Activity of PEDOT:PSS Film

Shuang Guo, Lei Chen[1,*], Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea
[1]*School of Materials Science and Engineering, Jilin Jianzhu University, China*

π-conjugated organic semiconductors with tunable electronic structures are new promising materials for surface-enhanced Raman scattering (SERS) active substrates. However, it is difficult to have high SERS activity due to the lack of plasmonic effect of hot electrons in organic semiconductors. Here, we designed an Ag-rGO composite structure and introduced it into poly(3,4-ethylenedioxythiophene) (PEDOT) in poly(3,4-ethylenedioxythiophene)-poly(tyrenesulfonate) (PEDOT:PSS) solution, and spin coated to form Ag-rGO/PEDOT:PSS film. Results of analysis show that the introduction of this Ag-rGO structure can not only enhance the electromagnetic field effect based on plasmon resonance, but also improve the interaction between the substrate and the probe molecule in Ag-rGO/PEDOT:PSS film. In this work, we not only improved the SERS activity of π-conjugated organic semiconductors, but also provided new ideas for the design of other organic semiconductor-based SERS substrates. The details of the mechanism will be discussed in this presentation.

Poster Presentation : **PHYS.P-163**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Chiral-induced Surface-enhanced Raman Optical Activity on Single-particle Level Substrate

Sung Gun Lee, Dae Hong Jeong*, SungJun Kwak[1]

Department of Chemical Education, Seoul National University, Korea

[1]*Science Education, Seoul National University, Korea*

Raman Optical Activity (ROA) has emerged as a valuable tool for characterizing stereostructural changes in both organic and inorganic compounds, offering complementary steric information to traditional spectroscopic methods. In particular, ROA has garnered attention as a chiral-selective method for analyzing biomolecules such as nucleic acids, and peptides, overcoming the limitations of conventional spectroscopy. However, due to the inherently low cross-section of ROA, which is three to five orders of magnitude lower than typical Raman, achieving sufficient signal sensitivity remains a challenge. To address this issue, efforts have been made to measure ROA signals using SERS, which utilizes plasmonic materials to enhance the Raman signal of analytes via the electric field concentrated around nanoparticles (SEROA). However, biomolecules typically have low Raman cross-sections and poor signal stability at high laser intensity and long measuring times, limiting the utility of SEROA. Recently, chiral-induced SEROA has been proposed as a breakthrough, leveraging the "sergeants-and-soldiers" principle to induce chirality in a trace chiral compound, enabling the measurement of chirality with shorter measuring times and lower laser intensities.This study demonstrates the use of a nanoparticle-on-mirror (NPoM) substrate and measurement configuration for SEROA, which isolates hotspots from particle aggregation. To confirm the reliability of the NPoM configuration for SEROA, chirality was induced in a self-assembled monolayer of 4-mercaptopyridine on a gold nanofilm surface. Furthermore, the mono-signate signal of the induced SEROA spectrum was shown to vary with the composition ratio of L/D-alanine, an inducer, confirming the correlation between chirality and SEROA signal.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Nanoscale Phase Behaviors of Binary Self-Assembled Monolayers Formed by Alkanethiols and Alkyl-substituted N-Heterocyclic Carbenes on Au(111)

Haeri Kim, Hyun Su Oh, Yeon O Kim, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) on metal substrates have been extensively studied due to their practical applications in fields such as nanoscience, biosensor, and electronic devices. Recently, N-heterocyclic carbenes (NHCs) with high chemical stability in solution or air have been proposed as new molecules instead of alkanethiol which has been studied over the past few decades. Binary SAMs are known as a helpful method to control surface and interface properties in the nanoscale. They are applied to various fields such as bio-interfaces and biosensors, electrical properties of molecular devices, and friction force control of surfaces. In this regard, we synthesized 1,3-dimethyl-5-(pentyloxy)-benzimidazolium hydrogen carbonate (C5-Me-NHC-HCO_3) and 1,3-diisopropyl-5-(pentyloxy)-benzimidazolium hydrogen carbonate (C5-iPr-NHC-HCO_3) to elucidate the wingtip effect on the formation and phase behaviors of NHCs and alkanethiols with different anchoring groups. We prepared binary SAMs by coadsorption method in a 1 mM THF solution with potassium tert-butoxide containing NHC and octanethiol (OT) as functions of molar ratios 10:90, 50:50, 90:10, and 95:5 at 50 °C for 1 h. The prepared SAMs were thoroughly investigated by using scanning tunneling microscopy (STM), cyclic voltammetry (CV) and X-ray photoelectron spectroscopy (XPS). In the binary SAMs of C5-Me-NHC and OT, our STM studies showed a heterogeneously mixed phase segregated stripped structure when the ratio of C5-Me-NHC was increased to 90%. On the other hand, binary SAMs of C5-iPr-NHC and OT formed a heterogeneously mixed phase when the NHC ratio was 50 %.

Poster Presentation : **PHYS.P-165**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

First-Principles Study of Co-free Li-excess ($Li_{1.25}Mn_{0.625}Ni_{0.125}O_2$) Layered Cathode Material

Joonkyung Jang*, Kisang Byun[1], Dohee Kim[1], Seyong Choi[1]

Department of Nanoenergy Engineering, Pusan National University, Korea
[1]*Nano Fusion Technology, Pusan National University, Korea*

Li-excess oxides have been regarded as a promising cathode material for next-generation Li-ion batteries due to their high energy density. Li-excess layered cathode materials are promising materials for novel positive electrodes with large capacities and energies compared to the state-of-art ones. From the structural point of view, these materials belong to the family of layered materials and can exchange large capacity at high operating voltages. In this study, we utilized first-principle calculations with VASP package to investigate the characterization of $Li_{1.25}Mn_{0.625}Ni_{0.125}O_2$. The structure was modeled by special quasirandom structures(SQS) method. By first-principle calculations, we obtained valuable information regarding the structural and electrochemical properties of $Li_{1.25}Mn_{0.625}Ni_{0.125}O_2$ layered material.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-166**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis of Styrene Carbonate: Computational Design and Evaluation of a Novel Ferrocene Catalyst

Wooram Lee, Joonkyung Jang[1,*], Seol Ryu[2,*]

nano fusion technology, Pusan National University, Korea
[1]*Department of Nanoenergy Engineering, Pusan National University, Korea*
[2]*Department of Chemistry, Chosun University, Korea*

We investigated the synthesis of styrene carbonate and proposes a novel ferrocene catalyst for this reaction. Styrene carbonate finds extensive applications in industries such as polymers and batteries, while also offering potential for carbon dioxide capture. The proposed catalyst with ferrocene, featuring two cyclopentadienyl rings surrounding an iron atom, incorporates two amines within its structure. Its unique composition endows the catalyst with dual Lewis acid and nucleophilic functionalities, suggesting high catalytic efficiency. Employing Density Functional Theory, the reaction mechanism was predicted and implemented, focusing on transition states that determine catalyst performance indicators like energy span and Turnover Frequency (TOF). Through computational calculations, this study aims to identify an efficient catalyst for styrene carbonate synthesis.

Poster Presentation : **PHYS.P-167**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Effects of Phase Separation on Protein Expression

Min Chung, Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

Intracellular phase separation has been getting a lot of attention due to its role in spatiotemporal compartmentalization of biomolecules. It has been suggested that compartmentalization of gene products via phase separation plays an important role in reducing the biological noises; indeed, it was experimentally shown that some liquid compartments could lower the range of fluctuations while maintaining protein levels. Using stochastic simulations, we analyzed the noise reduction effects of phase separation in protein expression. We found that upon phase separation, the noise in the protein concentration in any of the two phases was greatly reduced, and that the extent of noise reduction non-monotonically depends on the ratio between the amounts of genes present in the two phases. Our results suggest that the level of biological noise can be optimized via design and engineering of phase separation, and further studies will shine a light on the design principle of biological noise.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-168**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

In Silico Engineering of Binding Affinities of Green Fluorescent Proteins

Yu-Gon Eom, Jeong-Mo Choi[*]

Department of Chemistry, Pusan National University, Korea

Green fluorescent protein (GFP) has been used as one of the most effective agents for fluorescence microscopy. However, GFP has weak homodimerization binding affinity, which may interfere with the behaviors of fused proteins and thereby produce unwanted artifacts. Enormous efforts have been made to decrease the binding affinity of GFP homodimers, usually based on chemical intuition. Here, we utilized in silico methods to systematically mutate the interface of GFP homodimers and estimate the free energy changes. We first employed mmCSM-PPI, a machine-learning model for assessing changes in protein-protein binding affinity caused by single and multiple missense mutations, to rapidly check the binding affinity changes of all possible single-point mutations at the interface. We then collected the top most stabilizing and destabilizing mutations and carried out molecular dynamics simulations to estimate more accurate binding affinity changes, with the help of alchemical transformation methods. We found that the machine-learning approach and molecular dynamics simulations give generally correlated predictions but their predictions can be drastically different for some specific systems. We plan to experimentally assess the binding affinity predictions in the future.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Two-dimensional Ordering of Aromatic Thiol Self-Assembled Monolayers on Au(111) Guided by Displacement Method

Dongjin Seo, Haeri Kim[*], Hongki Kim[*], Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are ultra-thin films composed of organic molecules that are spontaneously adsorbed 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 forming SAMs. Aromatic thiol SAMs can affect the tail groups' reactivity and capacity to link to other species due to the extended π-system. Furthermore, the mechanical and thermal stability of aromatic SAMs is increased by irradiation-induced cross-linking. The high stability of cross-linked aromatic SAMs allows them to be used for nanolithography. In this study, we studied the structure and formation of benzene thiol (BT) and biphenyl-4-thiol (BPT). A previous study formed partially ordered BPT SAM at 50 ˚C EtOH 1 mM solution for 1 h. We used the displacement method in this study to form well-ordered BPT SAMs. Cyclohexane thiol (CHT) SAMs were used as a precovered layer in previous studies. CHT SAMs has axial and equatorial form of CHT, so it has large intermolecular distance. Intermolecular distance of 1-adamantanethiol (ADT) SAMs is wide (~ 0.7 nm) enough for BPT to be deposited. So ADT SAMs were also appropriate as a precovered layer. Ordered single ADT SAMs were formed at 50 ˚C EtOH 1 mM solution for 1 h in previous studies. In this study, we formed BT SAMs and BPT SAMs in EtOH 1 mM solution at RT for 30 min, 60 min, and 90 min to study the formation process. We obtained BT SAMs by displacement of CHT SAMs, and BPT SAMs by displacement of ADT SAMs. Subsequently, we used scanning tunneling microscopy (STM), cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS) to investigate prepared BT, BPT SAMs.

Poster Presentation : **PHYS.P-170**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Wingtip Group Effects on the Formation and Structure of Self-Assembled Monolayers of N-heterocyclic Carbenes with Alkyl Backbones on Au(111)

Yeon O Kim, Haeri Kim[*], Hyun Su Oh[*], Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Gold functionalized by self-assembled monolayers(SAMs) have important applications in microelectromechanical systems, surface protection, sensing and catalyst. In the prior research, thiol-based SAMs were investigated by many researchers. But despite their widespread use, thiols have a number of well-known drawbacks. Thiol-based surfaces have been seen to degrade significantly in a variety of environments, including ambient conditions, thermal treatment, and UV exposure. Due to these drawbacks, researchers found more robust replaceable SAMs for gold surfaces. Unlike thiol-based SAMs, N-heterocyclic carbene (NHC) SAMs have significant advantages including improved thermal, oxidative robustness, and resistance to pH changes. In this study, we used three kinds of benzimidazolium classes of NHCs, which are often referred to as standard carbenes, to make single component SAMs on Au(111). We synthesized 1,3-dimethyl-6-(pentyloxy)-1H-benzimidazolium hydrocarbonate (C5-Me-NHC-HCO_3), 1,3-diisopropyl-6-(pentyloxy)-1H-benzimidazolium hydrocarbonate (C5-iPr-NHC-HCO_3) and 1,3-dihexyl-6-(pentyloxy)-1H-benzimidazolium hydrocarbonate (C5-hex-NHC-HCO_3). For benzimidazolium NHC SAMs, the substituents attached to NHC molecules affect strongly to binding, mobility, stability, and characterization of gold surfaces. According to the recent study, the R-groups attached to the NHC nitrogen, colloquially referred to as wingtips, strongly influence the NHC's binding and orientation to the surface, while R' groups attached to the backbone modify the NHC's electronic structure and provide a modular binding site for targets. This research is aim to demonstrate wingtip effects of N-heterocyclic carbenes which have pentyloxy group for backbone.

Poster Presentation : **PHYS.P-171**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Molecular Self-Assembly of Aromatic Thiocyanates on Au(111)

Jun Hyeong Lee, Haeri Kim, Hyun Su Oh, Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are one common way to change the property of metallic surfaces since they are easy to prepare and modify while changing target molecules. In the last twenty years, lots of studies focused on fabricating Au(111) SAMs by using thiol analogues, but they are prone to oxidizing so changing headgroup to other compounds such as selenol analogues have been studied. There have also been reports about organic thiocyanates-based Au(111) SAMs that hardly oxidize and could form well-ordered SAMs on Au(111) while cyanate groups leave as a form of [Au(CN)2-] species. In this study, we used benzyl thiocyanate (BTC) molecules, which include thiocyanate groups as a headgroup to fabricate BTC SAMs. BTC molecules were obtained commercially and they were adsorbed on Au(111) in a 1 mM ethanol solution at room temperature and 50 ℃ condition. Benzenemethanethiol (BMT) molecules were also used to fabricate BMT SAMs in the same condition to figure out the affection of thiocyanate groups compared with thiol groups when forming SAMs. We characterized both BTC and BMT SAMs by using scanning tunneling microscopy (STM), cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS). Our STM-based surface analysis figured out that BTC and BMT SAMs could form ordered structures and our CV-based reductive desorption also revealed that both SAMs have reductive desorption peaks within the range of -900~-1,000 mV. Also, our XPS measurements showed that BTC SAM were formed via the chemical interactions between the sulfur anchoring group and Au(111) surface while cyanate groups leave when forming SAMs. To date, we fabricated BTC SAMs and compared them with BMT SAMs, which showed that BTC molecules could form well-ordered monolayers as in the case of BMT molecules.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-172**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

High Photocatalytic Effect of La/TiO_2/GO/Halloysite Nanocomposites for Degradation of Organic Dyes

Hongki Kim, Dongjin Seo, Haeri Kim, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

The purification of wastewater is a major issue in dealing with environmental problems. In this research, a novel nanocomposite, La/TiO_2/GO/Halloysite, is synthesized to enhance the photocatalytic degradation of environmental pollutants such as Rhodamine B. Halloysite, a naturally occurring aluminosilicate with a unique nanotubular structure, provides an ideal scaffold for the adsorption of pollutants. The combination of titanium oxide (TiO_2) and La^{3+} ion reduces the band gap and enhances the electron excitation of TiO_2 and results in a composite that exhibits photocatalytic activity in the visible region. Related research on La/TiO_2@HNTs showed that the adsorption amount of rhodamine B in La/TiO_2@HNTs was increased by 62% compared to TiO_2, and the photodegradation efficiency was increased by 36% for 20 min under UV irradiation and 16% for 2 h under direct sunlight. Integrating graphene oxide (GO) into this nanocomposite enhances its capacity to promote electron transfer, potentially leading to improved photocatalysis efficiency when decomposing organic pollutants. The structural, morphological, and functional characteristics of the synthesized La/TiO_2/GO/Halloysite nanocomposite is characterized using techniques such as XPS, XRD, and SEM. Using Rhodamine B as a model pollutant, this study aims to demonstrate the enhanced capability of the nanocomposite in decomposing organic dyes, paving the way for an efficient, cost-effective and renewable approach to wastewater treatment using solar energy.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Crossover between Energy and Charge-transfer in Two-Dimensional PTCDA/WS_2 Heterojunctions

Myeongin Song, Sunmin Ryu[*]

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

Two-dimensional (2D) semiconductors, represented by transition metal dichalcogenides (TMDs), have undergone extensively investigated due to their potential for electrical and optoelectronic applications. Heterostructures comprising highly crystalline 2D organic molecular crystals offer a broader range of possibilities compared to inorganic crystals, which have low absorbance and low tunability. In this work, we report on a confocal transient absorption spectroscopy setup optimized for 2D inorganic and organic semiconductors and interlayer excitonic behavior in their heterojunctions. For a higher sensitivity and flexibility on sample requirements, the change in absorption was obtained in the reflectance mode. The differential reflectance of 100-fs probe beam (330 ~ 1320 nm) was measured as a function of the time delay with respect to 140-fs probe pulses (520 nm). Furthermore, we investigated disparities in the IRF stemming from differences between refractive and reflective objective lenses. Additionally, we validated the transient reflectance (TR) signal of monolayer WS2 as a reference. Based on steady-state reflectance and photoluminescence of 1 to 4L PTCDA on 1L WS_2 samples, we identified the occurrence of inverted photoluminescence intensity trend above 4L PTCDA. This phenomenon could be emerged from the competition between distance-dependent charge and energy transfer processes.

Poster Presentation : **PHYS.P-174**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Circular Dichroism Spectroscopy of Jet-Cooled Amino Diphenyl Ethanol

Jiyeon Yun, Nam Joon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

We obtained the electronic circular dichroism (CD) spectra of jet-cooled amino diphenyl ethanol (ADE) near 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 ADE exhibited well-resolved vibronic CD bands. The IR-UV double resonance spectra showed that (1R,2S), (1S,2S)-ADE was present as several conformers in the jet. The magnitudes and signs of CD values of the vibronic bands varied depending on the types of the vibrational modes. These CD values can help to decide the chirality of each chiral center. The vibrational modes of each band were assigned by comparing the R2PI spectrum with the electronic spectrum computed considering the Franck-Condon (FC) and Herzberg-Teller (HT) contributions at the harmonic level. The rotatory strength values of each vibronic band were estimated using time-dependent density functional theory (TDDFT) calculations and compared with the CD values of the vibronic bands.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

A Study of Light-controllable Hydrogel using PEG and GFP for Insulin Delivery.

Namdoo Kim*, Su yeon Lim[1]

Division of Chemistry, Kongju National University, Korea

[1] *Kongju National University, Korea*

Hydrogel is a water-swollen network of cross-linked hydrophilic polymers. They are widely used as biomaterials for drug delivery, cell culture, and tissue engineering. Photo-dissociable dimeric Dronpa (pdDronpa) which is a GFP derivative, can be reversibly switched off/on and undergoes dissociation/association under the illumination of cyan/violet light, respectively. Such properties make it suitable for development of a light-controllable hydrogel, wherein pdDronpa serves as a photo-sensible crosslinker. Herein, we developed a photo-switchable hydrogel using 4-armed PEG-maleimide (M.W. 20K) and pdDronpa. The hydrogel underwent gel to sol transition upon cyan (500 nm) illumination, and returned to gel state upon violet (400 nm) illumination. In addition, the light-controlled insulin release was investigated using this hydrogel platform, showing that the release of insulin from the hydrogel to the environment can simply be controlled by adjusting pdDronpa dose and illumination time.

Poster Presentation : **PHYS.P-176**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Bioinformatic Analysis of Protein Structures Using Contact Map Formalism

TaeHwan Kim, Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

Structural information of a protein is the key to understanding its function. Therefore, vVarious experimental approaches have been developed to reveal determine protein structuresprotein structure information, leading to the construction of a database that contains hundreds of thousands of protein structures. The extensive database can be used Using these extensive databases, researchers have been working to uncover the principles governing protein folding and design. Previous studies have indicatedindicate 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 As a result, these CM-based measures cancalculations hold the potential to provide be used as a simple and efficient method proxy for evaluatingto evaluate the structural stability of proteins and, facilitating the *de novo* design and engineering of novel biomoleculeproteins in fields such as biotechnology and drug development.

Poster Presentation : **PHYS.P-177**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Towards Accurate Determination of Amyloid Fibril Stability Using Molecular Dynamics Simulations

Jeong-Mo Choi*, Taeseung Lee[1]

Department of Chemistry, Pusan National University, Korea

[1]*Chemistry, Pusan National University, Korea*

Amyloid fiber is a molecular feature of neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, and type 2 diabetes. Although the complete relationship of amyloid fibers to disease has not been identified, fiber stability has been suggested to be associated with pathological risks. Accurately estimating fiber stability, however, is indeed a challenging task in both computational and experimental investigations. In this study, we determined the fibril stability of amyloid beta using molecular dynamics (MD) simulations. We implemented an improved umbrella sampling method with additional collective-variable-based constraints and used it to obtain more accurate results compared to conventional methods. We anticipate that our improved method can pave a way to the full thermodynamic picture of the fibrillation of amyloid proteins.

Poster Presentation : **PHYS.P-178**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Mind the Gap: Energy Gap for Protein Binding

Chan-Gyu Kim, TaeHwan Kim, Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

Statistical mechanics of protein folding are governed 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 the first-order-like transition of folding. Inspired by the gap theory, the μ-potential has been developed to describe protein folding semi-quantitatively. 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.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-179**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Spatiotemporal carrier dynamics of pyrene incorporated multi-cation halide perovskites with high stability

Yu Jin Lee, Dongho Kim[1,*]

Yonsei University, Korea

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

Multi-cation mixed-halide perovskites, having remarkable optoelectronic properties, are emerging as photoactive layer materials for light-harvesting and light-emitting applicants. Improving the stability of these perovskite materials is the next hurdle for commercialization. Compositional engineering of cation sites and halide ion sites has been proven to improve phase stability. Pyrenes, being a planar conjugated system and a strong electron donor, is anticipated to passivate the defects at grain boundaries. The large size difference should allow the pyrenes to selectively locate in grain boundaries and interconnect the adjected grains through pi-conjugated bridges. This study observed further device stability enhancement by incorporating pyrene molecules in the precursor of Csx(FAPbI3)0.95(MAPbBr3)0.05 perovskites and spectroscopically unraveled the mechanism behind the improvement. Aided by confocal fluorescence lifetime imaging microscopy (FLIM), the distribution of photoluminescence (PL) lifetime and charge carrier diffusion dynamics were directly visualized in space and time in pyrene-incorporated multi-cation halide perovskites. Pyrene molecules were found to increase the diffusivity rate by a fold of 2 and therefore greatly improvethe diffusion length, proving that pyrene molecules assist the charge carrier transport effect by passivating the defects near grain boundaries. We also observed that the addition of pyrene precursors reduces the spatial energetic disorder at the perovskite surface. Furthermore, pyrene molecules Improved the overall stability when exposed to moisture. Perovskite films with pyrene addition showed no degradation in grain morphology and slower formation of nonradiative recombination sites near the grain boundaries.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-180**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

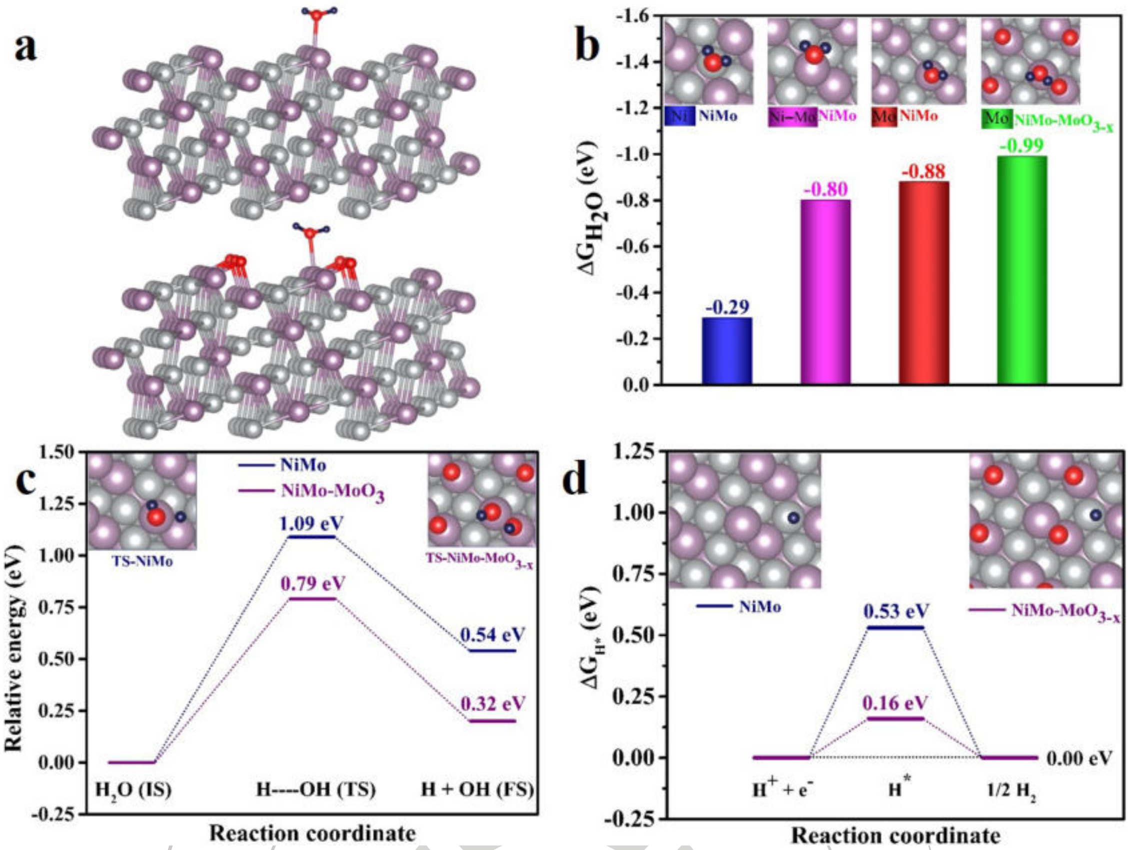
Computational Insights into Electrocatalytic Hydrogen Evolution: First-Principles Comparison between NiMo and NiMo-MoO_{3-x} Catalysts

Ramesh Kumar Chitumalla, Joonkyung Jang[1,*]

Institue of intelligent logistics big data, Pusan National University, Korea

[1]*Department of Nanoenergy Engineering, Pusan National University, Korea*

In the pursuit of efficient and sustainable energy sources, the electrocatalytic hydrogen evolution reaction (HER) stands as a crucial process for energy conversion. This study delves into a comparative analysis of NiMo and NiMo-MoO_{3-x} catalysts for their effectiveness in promoting the HER, employing a rigorous first-principles investigation. The catalytic performance of these materials is explored by examining their electronic structure, adsorption free energies of H_2O and H*, and reaction pathways of H_2O dissociation. By employing density functional theory calculations, we conclude that NiMo-MoO_{3-x} hybrid system is more favorable for HER kinetics compared to that of the NiMo. Our theoretical analysis provides valuable insights into the mechanistic aspects of HER, highlighting the underlying factors governing the catalytic activity of NiMo and NiMo-MoO3-x. The investigation sheds light on the potential of these catalysts in driving the electrochemical hydrogen evolution process, thereby contributing to the development of efficient and sustainable energy conversion technologies.


a
b
Ni NiMo
Ni–Mo NiMo
Mo NiMo
Mo NiMo-MoO3-x
ΔGH2O (eV)
-0.29
-0.80
-0.88
-0.99
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
c
TS-NiMo
NiMo
NiMo-MoO3
TS-NiMo-MoO3-x
1.09 eV
0.79 eV
0.54 eV
0.32 eV
Relative energy (eV)
1.50
1.25
1.00
0.75
0.50
0.25
0.00
-0.25
H2O (IS)
H----OH (TS)
H + OH (FS)
Reaction coordinate
d
NiMo
NiMo-MoO3-x
0.53 eV
0.16 eV
0.00 eV
ΔGH* (eV)
1.25
1.00
0.75
0.50
0.25
0.00
-0.25
H+ + e-
H*
1/2 H2
Reaction coordinate

Poster Presentation : **PHYS.P-181**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Efficient Detection of Cell Surface Proteins using a SERS-based Platform

Eungyeong Park, Sila Jin[1], Yeonju Park[2], Shuang Guo, Young Mee Jung[3,*]

Department of Chemistry, Kangwon National University, Korea
[1]*Department of Chemistry, University at Albany, SUNY, Albany, NY 12222, USA, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*
[2]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*
[3]*Department of Chemistry, Kangwon National University, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

Cell surface proteins play crucial roles in various biological processes and are closely associated with cell properties. As such, they serve as important biomarkers for disease diagnosis and the study of cellular processes. Despite many efforts to diagnose diseases, the development of an accurate diagnostic platform remains a challenge. In this study, we developed a platform for screening cancer-specific surface markers, such as epithelial cell adhesion molecule and E-cadherin, in both fixed and live cells using surface-enhanced Raman spectroscopy (SERS). Compared to other alternative methods, our proposed method using biocompatible antibody-conjugated SERS nanoprobes was successful in protein identification and quantification. In addition, this highly efficient SERS platform can be applied to the early diagnosis and prognosis of cancer and other biomedical applications.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-182**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Efficiency of FeCoNi-P/Co-OH Heterostructure Supported on Nickel Foam for Bifunctional Water Splitting

Mai Mai, Do hwan Kim[1,*]

Department of Energy Storage/Conversion Engineering, Jeonbuk National University, Korea
[1]*Department of Chemistry Education, Jeonbuk National University, Korea*

Transition metals have long been recognized as promising candidates in the domain of electrochemical catalyst research for water splitting. In this study, our endeavor involved crafting an interface engineering approach through the hydrothermal, and electrodeposition of Co-OH nanosheets connecting a FeCoNi phosphide heterostructure on a nickel foam substrate (designated as FeCoNi-P/Co-OH@NF). This architectural design serves the dual purpose of serving as effective electrodes for comprehensive water splitting in alkaline conditions. The incorporation of doped phosphorus (P) plays a pivotal role in achieving elevated valence states for alloys. This factor contributes to the enhancement of the oxygen evolution reaction (OER). Additionally, the P-doping significantly bolsters the efficiency of the hydrogen evolution reaction (HER), which can be attributed to the proximity of the d-band centers of the Ni atoms within the P-doped FeCoNi structure to the Fermi level. This proximity facilitates the adsorption and subsequent desorption of protons [1]. The integration of Co-OH nanosheets onto the surface of the nanorods has conspicuously ameliorated the catalyst's efficiency. Noteworthy is the observation that nanosheets, particularly when of reduced thickness, lead to a decrease in coordination numbers, an increase in surface-active sites, and the induction of defects. These combined effects contribute synergistically to heightened electrical conductivity [2]. For the FeCoNi-P/Co-OH@NF material, achieving a current density of 10 mA cm-2 in a 1.0 M KOH solution for both the HER and OER necessitated overpotentials of 100 mV and 300 mV, respectively. Impressively, this bifunctional electrocatalyst manifested cell potentials of 1.52 V in a 1.0 M KOH solution, and even after 100 hours of continuous operation, it displayed remarkable stability. Notably, these performance metrics outperformed

those of the commercial catalysts IrO2 and Pt-C. These findings introduce an innovative approach for fabricating electrolytic water electrolysis catalysts that excel in terms of cost-effectiveness, high performance, and stability in the field of hydrogen production.This research was supported by the Regional Leading Research Center Program (2019R1A5A8080326; 2022R1I1A1A01053248) through the National Research Foundation funded by the Ministry of Science and ICT of the Republic of Korea.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-183**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

DFT study of Ni and P doped MoS2 for the application of hydrogen evolution reaction (HER)

Phuong Le Thanh, Do hwan Kim[1,*]

Graduate School of Integrated Energy-AI, Jeonbuk National University, Korea

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

The oceans hold approximately 96.5% of Earth’s water, and seawater (SW) splitting provides infinite hydrogen sources with zero CO2 emissions while putting little strain on the Earth’s freshwater supply. Currently, benchmark commercial Pt/C is used for HER. Nevertheless, their rising price and scarcity are major obstacles to their practical implementation. Therefore, it is highly desirable to explore low-cost, efficient, and stable catalysts specially designed from earth-abundant metals for water splitting. The critical factors that can tune catalyst activity toward HER and water splitting[1]. For the development of efficient catalysts for the hydrogen evolution reaction (HER) by theoretical prediction, we examined Ni and P doped MoS2 slab/surface. The Ni/P-MoS2 surface phenomena were studied with the Vienna ab initio software package’s density functional theory (DFT), the calculations were simulated with the crystal parameters of GGA-PBE and Grimme’s DFT-D3 functions. The total density of states (DOS) was examined and shows the higher conductivity at the d-band centered Fermi level. Also, the optimized catalyst delivers lesser formation energy which proves that the catalyst was stabilized for further examination. So, this catalyst is further considered for hydrogen adsorption studies [2]. [Acknowledgement]: This work was supported by “Human Resources Program in Energy Technology” of the Korea Institute of Energy Technology Evaluation and Planning (KETEP), granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea. (No. 20204010600470).

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

DFT studies of nickel-cobalt phosphide carbon (NiCo3P-C) nanostructure for hydrogen evolution reaction (HER), Oxygen evolution reaction (OER), and Oxygen reduction reaction (ORR), as an efficient electrocatalyst

Saleem Sidra, Do hwan Kim[1,*]

Department of Energy Storage/Conversion Engineering, Jeonbuk National university , Korea

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

We investigated the catalytic activity of nickel phosphide (Ni2P), cobalt phosphide (Co2P), doping of Ni in cobalt phosphide [NiCoxP (x=1,2,3,4)], and nickel cobalt phosphide with carbon layer [NiCo3P.C] in hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR). The density of states (DOS) of NiCo3P.C around the Fermi level is significantly higher than Ni2P, Co2P, and NiCoxP (x=1,2,3,4) respectively, which indicates superior electrical conductivity to stimulate the catalytic activity. Among the possible reaction sites, P active site of NiCo3P.C has the lowest value of the Gibbs free energy of hydrogen adsorption (-0.158 eV), suggesting better HER activity. The calculated overpotential (η) in oxygen evolution reaction OER and oxygen reduction reaction (ORR) are 0.26 V and 0.21 V at P sites. These results represent that NiCo3P.C is a good trifunctional electrocatalytic material for HER, OER, and ORR applications. [Acknowledgement]: This research was supported by the Regional Leading Research Center Program (2019R1A5A8080326) through the National Research Foundation funded by the Ministry of Science and ICT of the Republic of Korea.

Poster Presentation : **PHYS.P-185**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Generative Deep learning for designing molecules with target optical properties in given solvents

Minhi Han, Joonyoung F. Joung[1], Sungnam Park[2,*]

Chemistry, Korea University, Korea

[1]*Department of Chemical Engineering, Massachusetts Institute of Technology, Korea*

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

We introduce a comprehensive deep learning framework that integrates predictive and generative models to design novel molecules with target optical properties. This approach enables the exploration of extensive chemical space, accelerating the discovery of new organic molecules and deepening our understanding of the relationship between molecular structure and optical properties. Our generative deep learning model, trained on a large experimental database, effectively generates molecules with specific properties such as absorption and emission wavelengths, bandwidths, extinction coefficients, fluorescence lifetimes, and quantum yields, even in regions with limited data. This integrated deep learning pipeline offers a promising tool for the efficient and targeted development of molecules in various fields, including organic photovoltaics, OLEDs, chromophores, and bio-imaging dyes, paving the way for the next generation of optoelectronic devices. The details and performance of our generative deep learning model will be presented.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-186**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Chemical vapor deposition of two-dimensional amorphous carbon

Jakub Wojciech Sitek, Maksim Rabchinskii[1], Pavel Bakharev[2], Marianna Sledzinska[3], Minhyeok Kim[4], Rodney Ruoff[5,*]

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Poland
[1]*Center of Multidimentional Carbon Materials (CMCM), Institute for Basic Science, Korea*
[2]*Center for Multidimensional Carbon Materials (CMCM) Institute for Basic Science (IBS), Korea*
[3]*Institut Català de Nanociència i Nanotecnologia, Institut Català de Nanociència i Nanotecnologia, Spain*
[4]*Chemistry, Institute for Basic Science/UNIST, Korea*
[5]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

Ultrathin amorphous carbon (aC) film is a novel two-dimensional (2D) material showing great promise as a 2D insulator for electronics applications.[1] In possible contrast to hexagonal boron nitride, it might be compatible with van der Waals heterostructures in which all processing is done by chemical vapor deposition.Our initial results suggest that our synthesized aC is a 2.5-nm-thick mechanically stable layer with a highly amorphous structure. The layer is electrically and thermally insulating, with a very low thermal conductivity of ~0.1 W/mK. Our current research efforts are focused on elucidating the growth mechanism by a parametric study involving temperature, pressure, times, and the CH_4/H_2 ratio. To try to understand the growth process in depth, we are comparing growth on two different monocrystalline substrates: Cu(111) and Ge(100). We are also studying some aspects of the film's structure by X-ray photoelectron spectroscopy. We are targeting enhancing basic science by understanding the nucleation of these aC films, and such further understanding might help (possibly) in its use as capping dielectric for electronic devices that are based on 2D materials.*We appreciate the support from the Institute for Basic Science (IBS-R019-D1). JS, a visiting scientist at CMCM, acknowledges the support from the NAWA Bekker Program (BPN/BEK/2022/1/00212).*[1] Toh, C-T.; Zhang, H.; Lin, J.; Mayorov, A.S.; Wang, Y.-

P.; Orofeo, C.M.; Ferry, D. B.; Andersen, H.; Kakenov, N.; Guo, Z.; Abidi, I.H.; Sims, H.; Suenaga, K.; Pantelides, S.T.; Özyilmaz, B. Nature 2020, 577 (7789), 199-203.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-187**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Charge-Transfer Absorption Band in Two-Dimensional PTCDA/TMDs Heterocrystals

Eunbeen Jeon, Sunmin Ryu*

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

Interfacial charge and energy transfer phenomena are widespread in both natural energy-harvesting organisms and artificial devices. Two-dimensional (2D) organic-inorganic (O-I) crystalline heterostructures offer a simple yet highly sensitive model system to study such interfacial transfer events. In this study, a 2D O-I system was fabricated using a physical vapor phase self-assembly deposition machine and its electronic structure was investigated using absorption and photoluminescence spectroscopy. Single and few-layer PTCDA (perylene-3,4,9,10-tetracarboxylic dianhydride), a representative organic semiconductor, was grown on 2D inorganic crystals of graphene and TMDs (transition metal dichalcogenides). A tubular physical vapor deposition system was built and tested for the growth of high-quality samples. The thickness and long-range order of PTCDA crystals were confirmed by optical contrast and polarized Raman spectroscopy, respectively. The absorption band observed at 1.7 eV likely results from ionized PTCDA molecules arising from O–I charge transfer. The mechanistic details of the charge transfer and its dependence on growth temperature will be discussed.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-188**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Theoretical investigation of photo and thermal reaction mechanisms of p-hydroxyphenacyl diethyl phosphate (HPDP)

Eunji Park, Joonghan Kim*

Department of Chemistry, The Catholic University of Korea, Korea

We examine the photochemical reaction mechanism of p-hydroxyphenacyl diethyl phosphate (HPDP) in solution using time-dependent density functional theory (TDDFT, MN12-SX/6-31G(d,p)) and multi-state complete active space second-order perturbation theory (MS-CASPT2). The calculated results show that the S_1 state of HPDP is populated and proceeds to the T_2 state via an intersystem crossing (ISC). Following this, the T_2 state of HPDP further progresses to the T_1 state through a conical intersection. Interestingly, these findings demonstrate a departure from prior theoretical results. The thermal reaction of HPDP occurs on the T_1 potential energy surface. The reaction intermediates, and transition states were identified using the DFT method (MN12-SX/6-31G(d,p)). The T_1 state of HPDP eventually proceeds to the S_0 state via additional ISC, which is optimized using the DFT method. This research represents the first investigation of the entire reaction mechanisms encompassing both photochemical and thermal reactions of HPDP. The comparison between the calculated results and the recent experiment is discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of density functional theory applicable to both absorption and fluorescence spectrum calculations with optimized van der Waals correlation functional

Dae-Hwan Ahn, Jong-Won Song*

Chemistry Education, Daegu University, Korea

In our previous study, we showed that LC-BOP with optimally tuned (OT) range separation parameter (μ) using Koopmans' theorem can accurately predict the absorption spectrum of conjugated systems with frontier orbital energies calculated in high accuracy [1]. However, OT-LC-BOP faces challenges when applied to systems where van der Waals interactions is important, such as excimer and exciplex, in that van der Waals correlation functional is not optimized to OT-LC-BOP with dynamically variable μ. In this study, we combine local response dispersion (LRD) method [2], which can calculate dispersion energy solely from the ground-state electron density, into LC-BOP with optimally tuned μ for high accuracy frontier orbital calculations (OT-LC-BOP+LRD). Therefore, considering that μ satisfying Koopmans' theorem varies depending on each system, we optimized the parameters of LRD for various μ values (0.16, 0.20, 0.30, 0.40, 0.47), respectively. We will also show that OT-LC-BOP+LRD can successfully reproduce not only the experimental absorption spectrum of previously tested excimers but also their fluorescence spectrum. [1] S. Jo, M. Ahn, K. Bhattarai, K. R. Wee, D.-H. Ahn and J.-W. Song, Chem Phys Lett, 2020, 761. [2] T. Sato and H. Nakai, J Chem Phys, 2010, 133.

Poster Presentation : **PHYS.P-190**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigation of photoswitching mechanism in single molecule localization imaging

Gaeun Go, Doory Kim[1,*]

Department of chemisty, Hanyang University, Korea

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

Super resolution microscopy (SRM) has emerged as a powerful tool that transcends the diffraction limits of conventional optical microscopes, enabling imaging of structures at the nanometer scale across various fields. Among various SRM techniques, single molecule localization microscopy (SMLM) employs stochastic conversion between fluorescent and dark states of fluorophores to acquire super-resolution images. In SMLM, it has been known that the formation of adducts between dyes and photoswitching reagents is vital for photoswitching phenomena of fluorescent dyes. While we understand how to create a dark state based on such an adduct, the mechanism for a reverse process remains unexplored. In this presentation, we propose a new mechanism for this fluorescence off-to-on conversion by studying the single molecule kinetics of Alexa fluor. Besides MEA, which is a representative thiol photoswitching reagent, we investigated other photoswitching reagents with diverse functional groups to propose a broader photoswitching mechanism. We could interpret the single-molecule kinetics data by comparing with the theoretical calculations, which could support our proposed photoswitching mechanism. We expect that our proposed photoswitching mechanism can not only provide the way for deeper understanding of photoswitching phenomena in SMLM imaging but also help in the further development of new photoswitching reagents.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-191**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of three-dimensional super-resolution imaging method for phase-separated polymer nanopatterns

DongMin Lee, Doory Kim[*]

Department of Chemistry, Hanyang University, Korea

Polymer lithography using phase separation is a valuable technique for nanofabrication and nanotechnology, offering nanoscale patterning capabilities, simplicity, versatility, and the potential for tailoring material properties to meet specific application requirements. It involves exploiting the phase separation of a polymer blend to create complex patterns and structures even at the nanoscale, which, however, are not observable by conventional light microscopes or electron microscopes. In this presentation, we propose a new strategy for the visualization of such a nanoscale polymer pattern formed by phase separation using super-resolution fluorescence microscopy (SRM). While SRM has predominantly found applications in biology through fluorescent labeling by immunolabeling or protein tagging, its utilization in organic or inorganic materials has been limited due to the lack of proper fluorophore labeling method. To overcome this limitation, we utilize the specific interaction between polymers and fluorescent dyes through functional groups. We demonstrate our method for three-dimensional super-resolution imaging of nanoscale patterned polymer formed by phase separation, which has not been achievable by conventional methods. Our new method allows detailed investigations of nanoscale phase separation in polymer blend film, which can potentially be used for further development of nanolithography.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of a low-field NMR spectrometer with an adjustable sample geometry

Minchae Kwak, Jung Ho Lee[1,*]

Chemistry, Seoul National University, Korea

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

Low-field NMR spectroscopy has emerged as a useful tool for molecular analysis, offering distinct advantages in terms of cost-effectiveness, portability, and ease of operation. We are developing a flexible low-field NMR system that can accommodate conventional cylindrical NMR tubes as well as fuel cells. To position the sample at the center of a bipolar magnet and to shield external RF noise, we have designed an optimized NMR probe frame. The computer-modeled probe frame was manufactured by CNC machining and 3D printing. To maintain B_0 field homogeneity, we have introduced shim coils in the NMR system. These coils generate magnetic fields that resemble spherical harmonic functions, which are orthogonal and can thus be combined to generate arbitrary magnetic field to compensate the B_0 field inhomogeneity. Shim coils and gradient coils were designed using an open-source electromagnetic simulation tool called bfieldtools to accommodate different sample geometries. Both the shim coils and gradient coils were fabricated on multilayer PCBs, which were attached to both sides of the probe frame. The probe assembly is compact and can be adjusted to sample geometry. Finally, we used the low-field NMR system to monitor an operating direct ethanol fuel cell (DEFC) in real time. We believe that continuous development and refinement of the NMR system will contribute to the understanding of fuel cell operation and aging.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

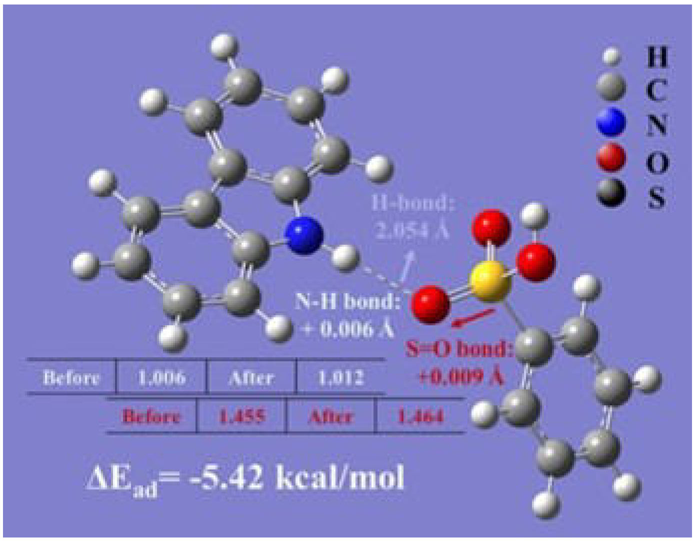
Exhibition Hall C THU 11:00~13:00

Removal of carbazole from model biodiesel composed of methyl laurate by using metal-organic frameworks functionalized with sulfonic acid both on metal and linker sites

Md Abul Hossain, Sung Hwa Jhung*

Department of Chemistry, Kyungpook National University, Korea

Although the content of organonitrogen compounds (ONCs) can be high, microalgae-derived esterified bio-oil can be an alternative energy source against the depletion of fossil fuel. Here, a metal–organic framework (MOF, MIL-101-NH_2, with or without grafting ethylenediamine, ED) was modified to derive sulfonic acid-functionalized MIL-101s. The obtained MOFs (including pristine MIL-101 and MIL-101-NH_2), together with activated carbon (AC) as a reference, were utilized in adsorptive denitrogenation (ADN), especially the removal of carbazole (CBZ), one of the most difficult ONCs via hydrogenation or oxidation, from model fuel composed of methyl laurate. Although there was a study on ADN from model fuel composed of very light esters like methylacetate, there is no report using esters that are quite similar to fatty acid methyl esters of oils. Remarkably, MIL-101-NH-ED-SO_3H, the first MOF having sulfonic acids on both the metal and linker sites, had noticeable maximum adsorption capacities (Q_o) for the stubborn CBZ removal although the porosity is the lowest among the studied adsorbents. For example, Q_o of the modified MOF was 205 mg/g which was higher than any studied adsorbents and was ca. 3 and 2 times that of AC and pristine MOF, respectively. The remarkable performance could be explained with H-bond (with a minor contribution of π-π interaction), based on calculations, FTIR, and functional groups of both the adsorbate and adsorbent. Furthermore, the recyclability of MIL-101-NH-ED-SO_3H in CBZ adsorption was confirmed. Therefore, MOFs when adequately functionalized can be useful in ADN of fuel composed of esters.


H
C
N
O
S
H-bond: 2.054 Å
N-H bond: + 0.006 Å
S=O bond: +0.009 Å
Before 1.006 After 1.012
Before 1.455 After 1.464
ΔE_{ad}= -5.42 kcal/mol

Poster Presentation : **PHYS.P-194**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Transient Absorption Microscopy (TAM), a Powerful Tool for Understanding Charge Carrier Dynamics.

Nohyoon Park, Jooyoung Sung[1,*]

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics and Chemistry, DGIST, Korea*

Conventional time-resolved spectroscopic techniques have been successfully applied to explore charge carrier dynamics in semiconductors. Nonetheless, these conventional methods often neglect morphology-dependent charge carrier behaviors. A novel spectroscopic technique, Transient absorption microscopy (TAM), has emerged as a promising method that facilitates the simultaneous observation of temporal and spatial behavior of charge carriers in morphologically complex materials. Here, we will describe our current TAM configuration and its diverse modalities. Our TAM setup has been meticulously designed to accommodate various operational modes. First, we integrated transmission and reflection geometries into the detection pathway, enabling comprehensive coverage across various semiconductor types with different sample thickness, surface quality, etc. Second, our TAM setup offers easy switching between confocal and wide-field beam modes, enabling us to capture charge carrier dynamics within local regions ranging from the Abbe deflection limit to several hundred micrometers. It is worth noting that combining different beam modes can extract photophysical properties such as transport length, diffusion coefficient, and more. Finally, an additional flexibility in our TAM setup is the capability to interchange the pump and probe beamlines. Although conventionally, the pump beam possesses higher energy than the probe beam, experimental requirements may necessitate a lower-energy pump beam. In such cases, the beamlines can be easily interchanged to suit the study's specific needs. While the aforementioned operational modalities are already integrated with our TAM setup, we are committed to further optimization of our TAM setup to achieve sub-ten femtosecond time resolution.

Poster Presentation : **PHYS.P-195**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Surface Accessibility of an Intrinsically Disordered Protein Probed by Laser-Assisted NMR Spectroscopy

Jonghyuk Im, Jongchan Lee, Jung Ho Lee[1,*]

Department of Chemistry, Seoul National University, Korea

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

Probing the protein surface accessibility of different residues is a powerful way to characterize the overall conformation of intrinsically disordered proteins (IDPs). Photochemically induced dynamic nuclear polarization (photo-CIDNP) is a phenomenon that occurs upon the transient interaction between a photo-excited dye and a surface-exposed aromatic residue. To quantitatively investigate the surface accessibility, it is necessary to perform time-resolved photo-CIDNP (TR-CIDNP) using a pulsed laser. However, it is challenging to illuminate short high-power laser pulses on NMR samples located inside the NMR magnet. Furthermore, only 1D TR-CIDNP experiments have been implemented so far in solution, and the low spectral resolution cannot provide residue-specific information for IDPs. Herein, we introduce several technical advancements to investigate the surface accessibilities of α-synuclein (α-Syn) using 2D TR-CIDNP experiments. High-energy laser pulses were transferred to NMR samples via an optical fiber, enabled by a pulse stretcher system. Ultrahigh-resolution 2D TR-CIDNP spectra were acquired by novel pulse sequences while maintaining sample integrity under multiple laser irradiations. Simultaneous application of radiofrequency and laser pulses enabled quantitative analysis of 2D TR-CIDNP. By applying these technical advancements, surface accessibilities of four tyrosine residues of α-Syn were measured to be nearly identical. Furthermore, conformational change of α-Syn induced by divalent cations was accurately investigated. The newly developed photo-CIDNP method can be used as an orthogonal and independent method of investigating important biological processes associated with the change of overall IDP conformation.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of nanoscale metrology and inspection tool for semiconductor using super-resolution fluorescence microscopy

Uidon Jeong, **Doory Kim**[1,*]

Department of Chemistry, Hanyang University, Korea, Hanyang University, Korea

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

Recent advancements in super-resolution fluorescence microscopy (SRM) have significantly enhanced the resolution of optical microscopes to the level of tens of nanometers. These advancements have not only extended the application of SRM to biological samples but also enabled its utilization in imaging polymer and semiconductor materials, thereby opening up new possibilities for nanomaterial imaging. In particular, super-resolution imaging and defect detection of nanopatterned semiconductors using the stochastic optical reconstruction microscopy (STORM) technique have been demonstrated recently. However, this method requires a polymer coating and fluorescent labeling process before STORM imaging, suffering from a significant tag size. In this presentation, we introduce our new technique that enables ultra-high-resolution fluorescence imaging without any such preprocessing steps. Our new approach not only achieves nanometer resolution for silica patterns but also enables non-destructive imaging without the need for the ultra-high vacuum required for electron microscopy. We anticipate that our novel technique holds the potential for application in imaging small circuit patterns created with EUV.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Improving Efficiency of Quantum Chemical Computations through Density Sensitivity of Atoms

Soohyeon Lee, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Recently, the role of quantum chemical computations for large-scale systems has become significant. However, applying relatively accurate computational methods is limited to small systems due to the high computational cost. To address this issue and enable efficient computation for large systems, embedding methods have been proposed. These methods divide the system into two main components: an important but small region, the active site, calculated by high-level methods, and the remaining area, the environment, calculated by low-level methods. Therefore, these methods are less computationally demanding than high-level methods for the entire system, but they are still more accurate than low-level methods alone. However, identifying the active site of a system is a challenge. In other words, it is not straightforward to know where the high-level method should be applied to get accurate results. There are many techniques to determine the active sites, but most require intuitive configuration of hyperparameters, such as the number of atoms in the active site or the active site itself. In this study, we introduce an efficient approach to automatically determine the active site, by calculating the impact of each atom on the overall reaction energy and using it as a criterion to define the active site. These impacts can be obtained from density sensitivity of each atomic orbital.

Poster Presentation : **PHYS.P-198**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Dispersion Corrections to Density-Corrected Density Functional Theory: DC^2-DFT

Minhyeok Lee, Mingyu Sim, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Semi-local density functional methods often fail to accurately depict long-range dispersion interaction. Within the Density-Corrected DFT (DC-DFT) context, every self-consistent DFT calculation has an error which can be categorized into functional and density-driven error. This study introduces a dual calibration approach for density-corrected DFT.[1] Firstly, we mitigate the density-driven error by density-correction using the Hartree-Fock (HF) density then correct the remaining functional error through dispersion adjustment, i.e., DC^2-DFT scheme. We explore various dispersion correction techniques, such as Grimme's DFT-D4[2], the exchange hole dipole moment (XDM)[3], and the many-body dispersion (MBD)[4]. Our insights underscore that for the success of DC^2-DFT methodology, the base functional chosen must lack inherent dispersion, allowing for the separate integration of omitted interactions. Additionally, incorporating HF density effectively addresses the pronounced delocalization error seen in standard DFT. Furthermore, it's essential to choose the training set for dispersion parameterization within the DC-DFT framework. Conforming to DC-DFT principles, our observations highlighted that every combination of the three dispersion correction methods with the selected functionals resulted in notable improvements in the dispersion interaction.[1] Suhwan Song, Stefan Vuckovic, Youngsam Kim, Hayoung Yu, Eunji Sim,* and Kieron Burke, Nat Commun, 2023, 14, 799. [2] Eike Caldeweyher, Sebastian Ehlert, Andreas Hansen, Hagen Neugebauer, Sebastian Spicher, Christoph Bannwarth and Stefan Grimme, J. Chem. Phys., 2019, 150, 154122.[3] A. Otero-de-la-Roza and Erin R. Johnson, J. Chem. Phys., 2019, 138, 204109.[4] Alexandre Tkatchenko, Robert A. DiStasio, Jr., Roberto Car, and Matthias Scheffler, Phys. Rev. Lett., 2012, 108, 236402.

Poster Presentation : **PHYS.P-199**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Photoluminescence Study of Two-Dimensional Picene Molecular Crystals

Hyunsuk Yun, Sunmin Ryu*

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

The study of excitonic behaviors in molecular crystals of reduced dimension has the potential to yield novel insights. Despite previous research on thin-film forms, it has proven challenging to obtain high-quality two-dimensional (2D) molecular crystals. In this study, we investigated the photoluminescence (PL) of 2D picene molecular crystals that were prepared via mechanical exfoliation on silicon wafer and physical vapor deposition (PVD) on graphene substrate. By mechanical exfoliation, we were able to obtain and characterize 2D picene crystals as thin as 15 nm using atomic force microscopy (AFM). Hence, by PVD, we were able to selectively obtain 2D picene crystals with thickness smaller than 5-layers and characterized and characterized their thickness using AFM and Raman spectroscopy. Upon excitation at 365 nm, we observed two vibronic bands for fluorescence and phosphorescence, centered at 390 and 500 nm, respectively. With decreasing thickness, the phosphorescence band became more prominent than the fluorescence band. This could be due to nonradiative decay channels, such as intersystem crossing or fluorescence quenching, for primary singlet excitons. Such effect could be elucidated by varying temperature and time-resolved spectroscopy experiments. We will discuss the possible role of each process and explore experimental methods to distinguish between them.

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Photophysical Studies of NIR Emitting Organic D-A Charge-Transfer Complexes

Jieun Bang, Jaehong Park[1,*], Juwon Oh[2], Sae Youn Lee[3], Chaewon Park[3]

Chemistry and Nanoscience, Ewha Womans University, Korea

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

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

[3]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Organic donor-acceptor (D-A) charge transfer complexes (CTCs) emitting in near-infrared (NIR) spectral domain have gained a lot of interest for biological imaging, optical communication, data storage, and night vision technology. The main goal of NIR CTCs development has been enhancing the radiative relaxation channel, enough to overcome their intrinsic small bandgap. Since the optical characteristics and excited state dynamics of CTCs are largely affected by their packing structures of each component, investigating structure-property relationships aiming rational design of CTCs is important. Here, we synthesized various CTCs based upon organic donors and acceptors with modulated packing structures by solution-phase methods as well as solid-griding methods. Steady state absorption and emission data showed CTCs were well formed. Time resolved fluorescence and transient absorption spectroscopy were utilized to investigate the molecular packing dependent excited state dynamics.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

NIR Photoluminescence Enhancement of Ag2S Nanocrystals by Chloride Passivation

Jiheon Kim, Juwon Oh[1,*]

Chemistry, Soonchunhyang University, Korea

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

Silver sulfide (Ag2S) nanocrystals have gained scientific attention in recent years based on their unique optical and electronic properties. Ag2S nanocrystals possess a narrow band-gap semiconducting materials (a band-gap for bulk Ag2S is ~ 1.1 eV), which allows that they can show photoluminescence in the short-wave infrared (SWIR) region, 900~1700 nm with a significant absorption cross-section. Furthermore, because they are non-toxic materials without cadmiums and leads, they have large possibilities for bio-applications. On the basis of these advantages, we studied NIR photoluminescence and electronic properties of Ag2S nanocrystals which are rich Ag-terminated. In addition, with a facile sonication treatment under a chloric-solvent environment, we verified that ligand exchange from alkyl amine to chloride results in an effective passivation and enhancement of NIR photoluminescence.

Poster Presentation : **PHYS.P-202**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

NIR Optical Properties of Surface-Controlled Ag2S Nanocrytals

Noh Yoona, Juwon Oh*

Department of Chemistry, Soonchunhyang University, Korea

Silver sulfide (Ag2S) nanocrystals have garnered significant attention in recent years owing to their distinctive optical and electronic attributes. These nanocrystals exhibit characteristics of a narrow band-gap semiconductor (with a bulk Ag2S band-gap of approximately 1.1 eV), enabling them to manifest photoluminescence within the short-wave infrared (SWIR) range of 900 to 1700 nm, accompanied by a substantial absorption cross-section. Additionally, their non-toxic nature devoid of cadmium and lead renders them highly promising for a diverse array of bio-applications. Recent intensive scientific efforts allow a surface control of Ag2S nanocrystals for a Ag-rich, S-rich, and stoichiometric Ag2S termination in the nanocrystals. These differently terminated Ag2S nanocrystals show distinct NIR emission properties and ligand exchange reactions, which results from their different trap states and their perturbation of core electronic nature.

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Adsorptive removal of 4-nitrophenol from water with covalent-organic framework derived nitrogen-enriched carbon.

Khan Md. Zubaed Hasan, Md Abul Hossain, Sung Hwa Jhung*

Department of Chemistry, Kyungpook National University, Korea

Continuous industrialization causes adverse impacts on human beings because of the contamination of water with toxic and undegradable organic contaminants such as phenolic compounds (PCs). Here, some nitrogen-rich carbonaceous materials, CDC(x)s, have been first prepared through the two-step carbonization of a covalent-organic framework SNW-1 (Schiff-based network-1). SNW-1 was pyrolyzed; the obtained product and potassium hydroxide mixtures were again pyrolyzed under different temperatures to get CDC(x)s. The carbonaceous materials were characterized and applied in the adsorptive elimination of para-nitrophenol (pNP, one of the representative PCs) from water. One CDC(x) called CDC(800) had a very high maximum adsorption capacity (Q_o), 1190 mg/g (at pH 7) which is 6 times that of activated carbon, and higher than that of any other known materials. Based on the adsorption results under various conditions, characteristics of CDC(800), and calculations, the plausible adsorption mechanism, such as hydrogen bonding (mainly between $-NO_2$ of pNP and H on the pyrrolic group of CDC(800)) and π-π interaction, could be suggested. Finally, the remarkable CDC(800) adsorbent was recyclable for several runs with ethanol washing; therefore, can be recommended as a competitive adsorbent to remove pNP from water.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Complete Basis Set Limit of HF-DFT

Byeongjae Kim, Eunji Sim*, Youngsam Kim[1]

Department of Chemistry, Yonsei University, Korea

[1]*Chemistry, Yonsei University, Korea*

Basis set extrapolation is a technique that aims to achieve large basis set calculation performance, using smaller basis sets.[1] By extrapolating calculated total energies with basis set size, we can attain complete-basis-set (CBS) limit thereby offering higher accuracy with reduced computational cost. HF-DFT, a nonvariational approach that combines Hartree-Fock density with DFT exchange correlation functionals as a pragmatic way of density-corrected DFT, provides an avenue for addressing errors in self-consistent DFT.[2] In this study, we investigated the behavior of HF-DFT when subjected to basis set extrapolation. In particular, we explore whether the total energies of molecules , and X fit with various extrapolation scheme. Also, we assess the extrapolation performance for reaction energies by benchmarking against W4-11, a subset of atomization energies from the GMTKN55 database.[3] Our findings reveal a linear relationship between total energy and X^{-3} in cc-pvXz and augcc-pvXz basis sets, with a mean R^2 value over 0.99. This implies that the CBS limit, extrapolated from double-zeta(X=2) and triple-zeta(X=3) basis sets, holds validity and can yield CBS reaction energies in most case. These results remain consistent across various functionals. We found CBS extrapolated energies can predict reaction energies better but this doesn't mean CBS limit is always better at every reaction in W4-11 set and it can differ by functionals, systems, and other factors.[1] Varandas, A. J. Annual review of physical chemistry, 2018, 69, 177-203.[2] Vuckovic, S., Song, S., Kozlowski, J., Sim, E., & Burke, K. Journal of chemical theory and computation 2019, 15(12), 6636-6646.[3] Goerigk, L., Hansen, A., Bauer, C., Ehrlich, S., Najibi, A., & Grimme, S. Physical Chemistry Chemical Physics, 2017, 19(48), 32184-32215.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-205**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

NMR Method Development for Selective Detection of Protein Acetylation

Kyungryun Lee, Sho Hee Park, Jung Ho Lee*

Department of Chemistry, Seoul National University, Korea

Acetylation regulates protein functions involved in essential cellular processes including gene expressions, protein-protein interactions, and enzymatic reactions. On the other hand, abnormal acetylation is related to various disease such as cancer and neurodegeneration. Therefore, determination of protein acetylation is important to predict protein behaviors in cells. We have developed an NMR pulse sequence, Ac-FIND (Acetylation-FIltered aNd eDited) to selectively detect signals arise from acetylated moieties. Based on the isotope editing and filtering technique, the sequence selects for the signals from specific combination ($^{12}\text{C}'(i–1)$, $^{12}\text{C}^{\alpha/\text{methyl}}(i–1)$, $^{13}\text{C}^{\alpha/\varepsilon}(i)$) of isotope resulted from acetylation. Thus, signal appears only when a protein is acetylated while no signal is observed for unacetylated proteins. Additionally, N-terminal and lysine side chain acetylation were able to discriminated by modulating excitation profile of E-BURP pulse incorporated in the sequence. For proteins with multiple lysine acetylation sites, acetylated lysine residues can be greatly resolved when combined with pre-homonuclear decoupling (PHD) scheme. We successfully validated applicability of Ac-FIND in vitro for intrinsically disordered α-synuclein and well-ordered ubiquitin by selectively detecting signals from acetylation after chemically acetylating both proteins using N-succinimidyl acetate. Furthermore, a single signal corresponding to intracellular N-terminal acetylation was observed by Ac-FIND when unacetylated $^{13}\text{C}/^{15}\text{N}$ labeled α-synuclein was introduced into live HEK293 cells. The results presented here demonstrate the usefulness of NMR method for detecting specific protein modifications in vitro as well as in cells.

Poster Presentation : **PHYS.P-206**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Transferability of HF-DFT to Periodic Systems

Youngsam Kim, Eunji Sim[1,*]

Chemistry, Yonsei University, Korea

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

Density Functional Theory (DFT) has emerged as a widely favored approach for solving electronic structure problems due to its reasonably high precision, and cost-effectiveness. However, the unknown exchange-correlation potential results in a variety birth of approximations and empirical parameters that lead to system-dependent accuracy. Meanwhile, DFT with the Hartree-Fock (HF) density has exhibited remarkable improvements in a variety of chemical reactions within cluster systems.[1] Unfortunately, the application of HF calculations in periodic systems proves to be computationally heavy due to the inclusion of non-local four-center integrals. The numeric atom-centered orbital with the Resolution of Identity method offers a promising route to mitigate the associated costs.[2] Since HF density is not an exact solution in density-corrected DFT schemes, and the success of clustered systems does not guarantee scalability to larger or periodic systems, many case studies are needed. In this study, we evaluate the performance of the recently developed HF-r2SCAN-DC4[3] through benchmarking databases and specific surface interaction. This result highlights the capabilities of the HF-r2SCAN-DC4 and further demonstrates its potential as a general-purpose tool for periodic system calculations.References[1] E. Sim, S. Song, S. Vuckovic, and K. Burke, J. Am. Chem. Soc. 2022, 144, 15, 6625–6639[2] S. V. Levchenko, X. Ren, J. Wieferink, R. Johanni, P. Rinke, V. Blum, and M. Scheffler, Comput. Phys. Comm. 2015, 192, 60-69 [3] S. Song, S. Vuckovic, Y. Kim, H. Yu, E. Sim, and K. Burke, Extending density functional theory with near chemical accuracy beyond pure water. Nat. Commun. 2023, 14, 799.

Poster Presentation : **PHYS.P-207**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Mechanisms of Carbonic Anhydrase and its Metal Variants through DFT Calculations

Rajeev Kumar, Jeong-Mo Choi[1,*]

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

Carbonic anhydrase (CA) is one of the most versatile metalloproteins which have been found from fish to humans in our animal kingdom. This zinc-based metalloenzyme catalyses the reversible hydration of carbon dioxide to form bicarbonate (HCO_3^-) and proton (H^+), thus playing a key role in pH and CO_2 homeostasis. Changes in CA activity are associated with various diseases such as glaucoma, type II diabetes, mellitus, and liver diseases. As CA is one of the most efficient enzymes (turnover frequency=10^6 s^{-1}) and also an important target for cancer therapy, a robust and clear understanding of the mechanism of carbonic anhydrase activity is very crucial. Here, we report our density functional theory (DFT) analysis on CA, comparing energetics of different structures obtained from high-pressure X-ray crystallography. We confirmed that the proton transfer reaction from water to hydroxide is a thermodynamically favourable reaction in the first step and then nucleophilic attack on carbon dioxide happens to form bicarbonate ion. As the central metal atom plays a crucial role in the activity of carbonic anhydrase, we also compared the variants of carbonic anhydrase containing Co^{2+}, Ni^{2+}, and Cu^{2+} and found that the coordination chemistry and consequent enzyme activity hugely depends on the identity of the metal.Reference:1.Jin Kyun Kim et al. “Elucidating the role of metal ions in carbonic anhydrase catalysis”, Nature Communication, 11, 4557 (2020).2.Denghui Ma et al. “Catalytic Coupling of CH_4 with CO_2 and CO by a Modified Human Carbonic Anhydrase Combined with Oriented External Electric Fields”, Organometallics, 39, 24 (2020).3.Björn Sjöblom et al. “Structural study of X-ray induced activation of carbonic anhydrase”, PNAS, 106, 26 (2009).

Poster Presentation : **PHYS.P-208**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Simulation Model for Percolation-Mediated Condensation of Associative Polymers

Da-Hyun Koo, Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

Biomolecular phase separation plays an important role in the formation and regulation of various biomolecular condensates in cells. Recently, the stickers-and-spacers framework, which is based on associative polymer theory, has been developed to explain the phase behaviors of biomolecules, and the framework was successfully implemented in a graph-based simulation module. The module uses the concept of percolation, which allows us to describe condensation in the language of graph theory, where percolation is depicted by the emergence of a giant component. We found that there are two relaxation processes, fast and slow; the former can be thought of as the initial formation of small clusters (proto-condensates or seeds), while the latter represents the growth of nuclei. We also analyzed the role of entropy loss due to sticker-sticker binding in condensation. Our study demonstrates that such a simple model can provide a qualitative understanding of a complex biological phenomenon.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Re-establishment of descriptor for hydrogen evolution reaction.

Jihoon Son, Hyeyoung Shin*

Graduate School of energy science and technology, Chungnam National University, Korea

Metal-hydrogen binding energy have widely used as a key descriptor for activity of hydrogen evolution reaction (HER). After first attempt was made by Norskov et al. which applied computational method to predict activity of HER, computational simulation has been widely used to predict HER activity of materials. However although HER takes place in electrochemical conditions, in most of case these conditions have not been taken into account. Hydrogen binding energy in solution phase condition is differ from gas phase, especially in some case of transition show reversed trend. In order to correct error caused by reaction condition and re-establish the descriptor of HER activity, we used implicit solvation model and compared adsorption energy of water with hydrogen on various surface facet and strain of Pt. Furthermore to reveal the exact reason that Pt show high activity on HER, for the materials which show adsorption of hydrogen in under potential region we investigated the hydrogen adsorption energy in different coverage and different site.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

A Miniature Reflectron Time-of-Flight Mass Spectrometer in the coaxial design

Kyu-Hong Kang, Eui-Young Ji[1], Kwang-woo Jung[2,*]

Physical chemistry / Department of Chemistry, Wonkwang University, Korea
[1]*Physical Chemistry/Department of Chemistry, Wonkwang University, Korea*
[2]*Department of Chemistry, Wonkwang University, Korea*

Development of a miniature reflectron time-of-flight (TOF) mass spectrometer is described on the based upon a coaxial arrangement. The instrument incorporates effusive beam of gas sample, electron ionization and a novel curved-field re¬flectron to maximize sensitivity and resolution over wide abundance and mass ranges. In addition, it includes the dual filament ion source and twin microchannel plate detectors to maximize mass spectrometer performance. Compared to previous designs, results indicate that resolution is improved, operating lifetime is extended, and the potential for mass producing this instrument in an inexpensive and rugged package for field-portable and remote installations is significantly enhanced. The technology will be adaptable to specific applications including real-time detection for hazardous chemical releases (e.g., chemical weapons), for environmental monitoring, and for process control in the semiconductor and display industry.

Poster Presentation : **PHYS.P-211**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Electron Beam Cross-Linking Mechanism of Cyclotetrasiloxane-Based Inorganic Molecular Resists for EUV Lithography

Jiyoung Bang, Hyeok Yun[1], Wonchul Kee[1], Hyun-Dam Jeong[1,*]

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

Next-generation extreme ultraviolet lithography (EUVL) is an essential technology for miniaturization of semiconductors. However, it is necessary to develop an optimized EUV resist due to a different exposure mechanism than before. Inorganic resists have attracted considerable interest in EUVL applications due to their high mechanical strength and etch resistance. In this study, tetrahydroxy-tetramethyl-cyclotetrasiloxane (tetraol) was used as EUV and electron beam resist. The electron beam sensitivity (D_{50}) was 21.9uC/cm^{-1} and the EUV absorption coefficient was 9.89 cm^{-1}. In EUVL, a photoresist film was formed with a 22 nm HP pattern at 55 mJ/cm^2. It also showed 65.4 times higher etch resistance than spin-on-carbon (SOC) because of its rigid siloxane core. The electron beam exposure area was analyzed using FT-IR, XPS, and TOF-SIMS to investigate the cross-linking mechanism of tetraol upon electron exposure. The presence of silanol groups in the material promotes cross-linking, leading to increased sensitivity during electron beam exposure. Additionally, we also confirmed the potential for radical reactions through the cleavage of Si-C bonds, in addition to the cross-linking of the silanol group. Furthermore, to enhance the EUV absorption coefficient, we introduced tin into the siloxane core.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Enhanced photocatalytic degradation of toxic dyes with core-shell nanoparticle clusters

You Hee Seo, Jeongmin Seo[1], Chaeyoung Im[1], Seunghoon Lee[*]

Department of Chemistry, Dong-A University, Korea

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

Colloidal clusters composed of core-shell nanoparticles (NPs) with plasmonic core and catalytically active shell offer a promising platform to combine catalytic reactivity and enhanced plasmonic performance for visible light photocatalysis. We reported a novel synthetic strategy for the nanoparticle clusters (NPCs) in aqueous solution through fine controlled galvanic replacement between Ag nanoprisms and Au precursors. These model systems allow us to study the synergy effect of hot spots and bimetallic composition in plasmonic catalysis. In this study, we explore the influence of electromagnetic hot spots in core-shell Au@M (Pd or Pt) NPCs to induce efficient energy transfer for degradation of various dyes under LED solar simulator illumination. Hotspots, a strong electromagnetic field generated from the interparticle gaps of Au NPCs through the interaction of light with NPs, increase catalytic efficiency, allowing the drastic degradation of various dyes. In addition, the Pd or Pt used as a catalytically active shell has a stronger degradation effect alongside the hot spots of the Au NPCs due to its outstanding catalytic properties of distinctive electronic configuration and surface reactivity. These findings have significant implications for the design and synthesis of hybrid nanomaterials with enhanced plasmonic and catalytic properties for applications in wastewater treatment and environmental improvement.

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of clustering analysis method for single-molecule localization images

Hyungjun Lim, MinJeong Kim, Hui Chong Lau[1], Sung-Soo Park[1], Doory Kim*

Department of Chemistry, Hanyang University, Korea

[1]*MDimune, Korea*

Recently, various super-resolution microscopy (SRM) techniques have been developed to overcome the diffraction limit of light microscopy. As a representative SRM, stochastic optical reconstruction microscopy (STORM) can obtain super-resolution images through the acquisition and reconstruction of fluorescence signals from single molecules. Consequently, each fluorescence signal from single molecule in STORM image generates precisely localized coordinate, which is used to reconstruct the final super-resolution image. Since the STORM image is reconstructed from individually localized points obtained by the detection and localization of single fluorescent molecules, this high-resolution image reveals a pointillistic nature and requires a new method for cluster analysis. Traditional clustering analysis has been developed mainly for intensity grid-valued pixel-based images obtained from conventional microscopy. Therefore, this methodology has not been successfully applied to pointillism STORM image. To overcome this limitation, we develop a novel clustering analysis method for STORM images by using density-based spatial clustering method and AI clustering model. We successfully demonstrated this novel method for analyzing super-resolution images of cell-derived vesicles in various sizes. We expect that our methods can clarify demanding questions in a wide range of biology by providing ultrastructural information about targets, finally playing a significant role in super-resolution image analysis.

Poster Presentation : **PHYS.P-214**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Why and How to Increase EUV-Induced Material Alteration Degree in EUV Inorganic Resists? : The Effect of Electron Beam Irradiation on Dibenzyltin Diacetate Thin Film Using Local Analysis and Quantum Chemical Calculations

Hyeok Yun, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

When exposed to extreme ultraviolet (EUV) light, photoresist (PR) molecules produce secondary electrons. These electrons then interact with nearby molecules, causing reactions like neutral dissociation, dissociative ionization, and dissociative electron attachment, leading to a chemical contrast in the PR.A PR's EUV-induced material alteration degree (EUV-MA) indicates a 'chemical alteration degree' regardless of development conditions. This EUV-MA significantly impacts two important steps in the photolithography process: the expression of the PR's chemical contrast upon exposure, and the refinement of the manifested chemical contrast through development conditions. Maintaining a high EUV-MA while using strong development conditions is optimal approach to enhance the performance of a PR.To estimate the EUV-MA of a PR, one must investigate the changes in the molecular structure of the PR before and after exposure to EUV. However, the limited accessibility of EUV light sources is a constraint in the study. Based on the strong similarity in the energy distribution of secondary electrons from both electron beam (E-Beam) and EUV, we can use E-Beam as an alternative to EUV. The reaction of dibenzyltin diacetate thin films under E-Beam irradiation was studied with local analysis techniques using FT-IR, TOF-SIMS, and XPS. Through this, we demonstrated that not only the benzyl group but also the acetate group in dibenzyltin diacetate molecules can undergo dissociation. Additionally, through the natural bond orbital analysis of the dialkyltin dicarboxylate series, we computed the difference in bonding-antibonding orbital energies of Sn-C and established the relationship between their molecular structure and EUV-MA.

Poster Presentation : **PHYS.P-215**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Synthesis and Characterization of Zinc-Oxo Cluster for EUV and E-beam photoresist

Jiyoung Bang, Hyun-Dam Jeong[1,*]

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

Zinc oxo clusters (ZOC), which exhibit a relatively high EUV absorption cross-section, have garnered attention as potential EUV photoresist materials due to their high EUV sensitivity. Carboxylates are commonly employed as ligands in EUV photoresists, as they undergo decarboxylation during EUV exposure, enabling reactions. Additionally, fluorine-rich compounds, such as fluorine, exhibit higher EUV absorption cross-sections compared to hydrogen, leading to increased EUV absorbance when incorporated as terminal groups. Furthermore, zinc oxo clusters with functionalizable benzoate ligands offer the potential for molecular bridging through EUV or electron beam exposure, exhibiting negative-tone photoresist characteristics. Prior to conducting the study, trifluoroacetate zinc oxo clusters were heated to 50°C with benzoic acid and a minimum amount of acetone anhydrous. The resulting mixture was then stored below 0°C for several days to obtain a solid. As a result, a zinc benzoate oxo cluster (ZBOC) was synthesized by replacing trifluoroacetate (TFA) with benzoate.

Poster Presentation : **PHYS.P-216**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Basis Set Superposition Error and Counterpoise Correction in Hartree-Fock DFT

Se hun Kim, Youngsam Kim, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Basis set superposition error (BSSE) is one of the prominent errors in computational chemistry, caused by nuclear-fixed basis sets. It occurs when one monomer within a dimer utilizes the basis set of another monomer, leading to a calculated energy that is lower than the actual energy. This error mainly causes problems in calculations involving noncovalent interactions such as hydrogen bonding and van der Waals complexes. Counterpoise (CP) correction can reduce BSSE and its effectiveness has been extensively investigated for correlated wavefunction methods and self-consistent density functional theory (DFT). Its application to density-corrected DFT (DC-DFT), however, remains largely unexplored. In this work, we have performed calculations within self-consistent DFT and Hartree Fock-DFT (HF-DFT), a practical DC-DFT procedure, by varying basis set and approximate density functionals. As a result, we have found that the properties and trends of CP corrections in self-consistent DFT also hold for CP corrections within HF-DFT.

Poster Presentation : **PHYS.P-217**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Electrochemical Performance of π-Conjugated Molecule Bridged Silicon Nanocrystal Nanocomposite Synthesized by Imine Conjugation Reaction for Lithium-Ion Battery Anode Material

Minyeop Kim, Soyeong Heo[1], Hyun-Dam Jeong[2,*]

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

π-Conjugated molecule bridged silicon nanocrystal nanocomposite (Si NCNC) was prepared by imine conjugation reaction between 4-hydroxybenzaldehyde and octanol co-capped silicon nanocrystals (4-Hb/Oct Si NCs) and 4-aminophenol and octanol co-capped silicon nanocrystals (4-Ap/Oct Si NCs). The chemical properties of the Si NCNC were confirmed by Fourier transform infrared spectroscopy, field emission transmission electron microscopy. The 4-Ap/Oct Si NCs and the Si NCNC were used as anode materials of lithium-ion batteries to investigate the effect of clustering on the electrochemical performance. The π-conjugated molecules between Si NCs serve as a buffer layer to relieve the mechanical stress arising from the alloying reaction of lithium and Si and maintain the electrical conduits in anode system, improving the electrochemical performance of Si NCNC.

Poster Presentation : **PHYS.P-218**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Electrochemical Performance of π-Conjugated Molecule Bridged Silicon-Silver Nanocrystal Nanocomposite as Anode Materials for Lithium-Ion Batteries

Seong-Gun Lee, Minyeop Kim[1], Hyun-Dam Jeong[*]

Department of Chemistry, Chonnam National University, Korea

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

In lithium-ion batteries, silicon-based anode materials exhibit the issue of volume expansion during lithiation and volume contraction during delithiation cycles, leading to the formation of pulverization. This problem can be overcome by synthesizing π-Conjugated molecule bridged silicon nanocrystal nanocomposites (Si NCNC), which connect the silicon nanocrystals and formation due to mechanical stress. Additionally, there is a challenge of decreased charge-discharge capacity at high C-rates, which is addressed by improving electrical conductivity through the hybridization of highly conductive silver nanocrystals and silicon nanocrystals. Firstly, we synthesized 4-hydroxybenzaldehyde and octanol co-capped silicon nanocrystals (4-Hb/Oct Si NCs), 4-aminophenol and octanol co-capped silicon nanocrystals (4-Ap/Oct Si NCs), and silver nanoparticles capped with cysteine. The synthesized materials were characterized using fourier transform infrared, high-resolution X-Ray diffractometer and field emission transmission electron microscopy. These materials were mixed and used as anode materials for electrochemical property analysis, which was conducted and compared.

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Impact of Solvent Environment on Singlet Fission Rate in Perylene Bisimide Dimers

Jonghwan Lee, Daniel Yim, Sunghwan Choi[1,*], Hyungjun Kim[*]

Department of Chemistry, Incheon National University, Korea

[1]Korea Institute of Science and Technology Information, Korea

Singlet fission(SF) is the intriguing photophysical process that the lowest singlet state(S_1) generated by some external stimulus like light is converted into two independent triplets, intermediating a multiexciton state(ME), which is a promising phenomenon for the photovoltaic systems as the quantum yields can be increased up to 200%. It is widely known that there are three possible SF mechanisms : (1) Two-step pathway that charge-transfer(CT) state presents the intermediate between S_1 and ME, (2) Superexchange pathway that CT state populates as virtual, not real, to boost the electronic coupling (3) Direct pathway that there is no CT state involvement in the SF process. So understanding the role of CT state is significantly essential for the SF mechanism.Recently, restricted active space with spin-flip(ras-sf) methods are well introduced for calculating not only the energy level of the singly excited state but the one of the doubly or more excited state containing spin-flip. However, ras-sf has the critical weakness that it cannot describe a dynamic correlation of electrons and a solvation effect simultaneously and it can be partially covered through DFT empirical correction.Recent studies show the importance of solvent impact on SF. For example, the experimental results indicate that the SF rates of Bis-PBI, which is perylene bisimide dimers linked by binaphthyl group, are faster as the solvent polarity becomes higher. But ras-sf cannot calculate it as it assumes the gas phase condition.In this research, we calculated the SF rates of Bis-PBI considering the solvation effect. Through this studies, we tried to understand the relationship between SF and the polarity in the molecular perspective.

Poster Presentation : **PHYS.P-220**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Pre-Homonuclear Decoupling: NMR Measurements of Intrinsically Disordered Proteins at Ultrahigh Resolution

Sohyun Jung, Jonghyuk Im, Kyungryun Lee, Jung Ho Lee[1,*]

Department of Chemistry, Seoul National University, Korea

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

Intrinsically disordered proteins (IDPs) carry out important functions in cells and are related to the pathogenesis of many neurodegenerative diseases. To analyze IDPs, it is necessary to resolve different NMR signals generating from IDP residues. Although NMR signals from IDPs are generally sharp and strong, some of them tend to substantially overlap. In this work, we present a new homonuclear decoupling scheme called Pre-Homonuclear Decoupling (PHD). The PHD method does not apply radiofrequency pulses and pulsed field gradients during the FID period, but is rather based on the in-phase/antiphase (IPAP) principle. This method uses a narrow distribution of 1JCαHα coupling values to decouple 3JHNHα couplings between amide (1HN) and alpha (1Hα) protons. First, we applied PHD to the 2D 1H-15N heteronuclear single-quantum coherence (HSQC) to obtain 3-fold narrower 1HN line widths compared with the control HSQC for the alpha-synuclein (α-Syn) sample. Next, we applied PHD to the transverse relaxation-optimized spectroscopy (TROSY). TROSY-based experiments generally possess narrow 15N line widths, but are affected by the 3JHNHα couplings in the 1H dimension. By labeling the longitudinal spin order of an α proton (Hαz) on multiple quantum coherences of backbone nuclei, the PHD-TROSY provided ultrahigh resolution in both 1HN and 15N dimensions as demonstrated in the analysis of Tau. We also designed 3D HNCA with the PHD-TROSY readout, which assigned all amide resonances of α-Syn using a single experiment. In summary, the PHD scheme provided narrow 1HN line widths with minimal artifacts for high-resolution analysis of IDPs.

Poster Presentation : **PHYS.P-221**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Tin Oxo Cluster Photoresist CNU-TOC-01(4C-C) for Extreme Ultraviolet (EUV) Lithography

Hyeok Yun, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

The molecular structure and lithographic characteristics of a tin oxo cluster photoresist, referred to as CNU-TOC-01(4C-C), were investigated. The structure of CNU-TOC-01(4C-C) was inferred using field desorption time-of-flight mass spectrometry, and its average diameter was determined to be approximately 1.3 nm via dynamic light scattering. A coating solution of CNU-TOC-01(4C-C) was prepared by dissolving it in ethyl lactate at a concentration of 5 wt%. Thin film fabrication was performed by spin-coating the solution onto a 100 nm SiO_2/Si wafer at 3000 rpm for 30 s. Patterning was carried out using either an electron beam(E-beam) or extreme ultraviolet(EUV) radiation. Post-applied bake and post-exposure bake were performed identically at 180°C for 5 min and 190°C for 5 min, respectively. Following the post-exposure bake, each film was developed in a 2.38 wt% tetramethylammonium hydroxide solution for 10 seconds. The D_{50} and contrast of CNU-TOC-01(4C-C) for E-beam square patterning were 514.3 $\mu C/cm^2$ and 8, respectively. A 22 nm half-pitch pattern was observed at 105 mJ/cm^2 dosage in EUV line patterning.

Poster Presentation : **PHYS.P-222**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Density-Corrected DFT for Molecular Properties: Dipole Moment

Jiye Shin, Mingyu Sim, Soohyeon Lee, Youngsam Kim, Eunji Sim[*]

Department of Chemistry, Yonsei University, Korea

Density Functional Theory (DFT) has greatly developed the field of quantum chemistry by allowing scientists to analyze molecular systems and predict their properties while balancing computational efficiency and accuracy. The dipole moment represents the overall charge distribution of a molecule and is a key descriptor of its polarity. Numerical methods used to determine the dipole moment in an electric field have been well studied. Still, DFT calculations may not be accurate in certain systems, such as BS, HCCF, and NaLi. This study validated the results of previous papers that density corrected DFT is effective in reducing energy errors and yielding accurate dipole moments, and further investigated its performance in HF-r^{2}SCAN. We also see the effect of the dispersion correction on the dipole moment as a response to energy.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-223**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

De novo nanobody binder design by generative AI models

Hakyung Lee

Molecular Medicine and Biopharmaceutical Sciences, Seoul National University, Korea

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-224**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Absolute determination of crystal orientation by phase-resolved SHG spectroscopy

Jihun Kim, Sunmin Ryu[*]

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

Two-dimensional materials like graphene are characterized by distinct layering and bonds formed through weak van der Waals forces. Among them, transition metal dichalcogenides (TMDs) stand out due to their band gap and exceptional electronic properties, which are influenced by stack angles. Consequently, analyzing the crystal orientation angle of TMD materials is crucial for applications. Traditional methods, such as using the intensity properties of polarized Second Harmonic Generation (SHG), face difficulties when dealing with MoS2 monolayers exhibiting flipped geometries [1]. In response to this challenge, our research focuses on the phase properties of monolayer TMDs [2]. Through this, it was possible to find out the absolute orientation of the monolayer TMDs. We further quantified the phase difference across various TMDs and explores into the orientation-specific chemical reactions of MoS2. Our groundbreaking approach introduces a trustworthy and non-invasive method for determining crystal orientation, expecting advancements in TMD research and applications.

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Rotational Isomerization of Carbon-Carbon Single Bonds in Haloethyl Radicals in Solution

Seongchul Park, Juhyang Shin, Hojeong Yoon, Manho Lim*

Department of Chemistry, Pusan National University, Korea

The rotational isomerization of 1,2-disubstituted ethyl radical derivatives, reaction intermediates often found in the reaction of 1,2-disubstituted ethane derivatives, has never been measured because of their short lifetime and ultrafast rotation. However, the rotational time constant is critical for understanding the detailed reaction mechanism involving these radicals, which determine the stereoisomers of compounds produced via the intermediates. Using time-resolved infrared spectroscopy, we found that the CF2BrCF2 radical in a CCl4 solution rotationally isomerizes with a time constant of 47 ± 5 ps at 280 ± 2 K. From this value and the rotational barrier heights of related compounds, CH3CH2 and CH3CH2CHCH3 radicals in CCl4 were estimated to rotationally isomerize within 1 ps at 298 K, considerably faster than ethane and n-butane, which rotationally isomerize with time constants of 1.8 and 81 ps, respectively. The time constant for the rotational isomerization was similar to that calculated using transition state theory with a transmission coefficient of 0.75.

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Rebinding Dynamics of Carbon monoxide with Cytoglobin Using Time-resolved Infrared Spectroscopy

Juhyang Shin, Manho Lim[*]

Department of Chemistry, Pusan National University, Korea

Time-resolved vibrational spectroscopy was used to probe the rebinding dynamics of CO to cytoglobin (Cgb) after photodeligation of the corresponding CO-bound protein in D_2O at 273 K. When excited with a 532-nm photon, carbon monoxide dissociated immediately from cytoglobin (< 0.2 ps), ground state bleaching of CO bound to the cytoglobin has three conformations (A0, A1 and A3). Each conformation shows characteristic $^{13}C{-}O$ stretching frequencies. The vibrational spectrum of CO in Cgb^{13}CO described three gaussians at 1924.6 cm^{-1} (A0), 1900.2 cm^{-1} (A1) and 1884.5 cm^{-1} (A3) with a full width at half-maximum (FWHM) of 16 cm^{-1}, 15.8 cm^{-1} and 12.5 cm^{-1}. Ligand binding to Cgb is a multiphasic process with fast geminate rebinding taking place on the nanosecond timescales and slower biomolecular rebinding occurring on microsecond timescales.

Poster Presentation : **PHYS.P-227**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Advancing Spectral Analysis: Two-photon IR+VUV-MATI Technique for Resolving Low-frequency Vibrational Modes in Thietane

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

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

[1]*Forensic Chemistry Division, National Forensic Service, Korea*

Observing and analyzing low-frequency vibrational modes, such as the ring-puckering mode in thietane, presents significant challenges. The presence of these low-frequency, large-amplitude vibrational modes can result in a more intricate spectrum. The overlap of various vibrational modes adds complexity to assigning specific vibrations to the observed peaks in the one-photon VUV-MATI spectrum. To overcome these challenges, a two-photon IR+VUV-MATI spectroscopic technique has been adopted. This innovative approach combines infrared (IR) radiation with vacuum ultraviolet (VUV) radiation for ionization. This technique capitalizes on the vibrational peaks in the C-H region of neutral thietane. The ultimate goal is to compare the outcomes obtained from the two-photon IR+VUV-MATI spectroscopy with those from the one-photon VUV-MATI spectrum. This comparative analysis is expected to illustrate how the new technique can effectively simplify the spectral complexity and offer clearer insights into the vibrational modes, including the intricate ring-puckering mode. The findings and methodology will be presented through a poster presentation. This platform is likely to highlight the advantages and benefits of the two-photon IR+VUV-MATI technique in streamlining spectral interpretation, ultimately contributing to a deeper understanding of molecular behavior and conformation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-228**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Spatial Correlation in Dynamics of Glassy Polymers

Park Joohyeong, Hyun Woo Cho*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

In this study, we carry out extensive molecular dynamics simulations with employing bead-spring polymer model, in order to investigate the sluggish and heterogeneous dynamics of glassy polymer melts. We estimate structural relaxation of polymers using the self-part of the time-dependent overlap function, and quantify the magnitude of dynamic heterogeneity using its fluctuations. By examining the four-point dynamic structure factor, we identified the size and morphology of the dynamically correlated regions. As the temperature approaches the glass transition point, the size of these regions grows. Notably, below the dynamic transition temperature, the morphology of these regions transitions from fractal to compact. These patterns mirror those in glassy liquids composed of spherical particles, such as metallic and colloidal glasses, affirming the universal nature of heterogeneous dynamics in glassy materials.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-229**

Physical Chemistry

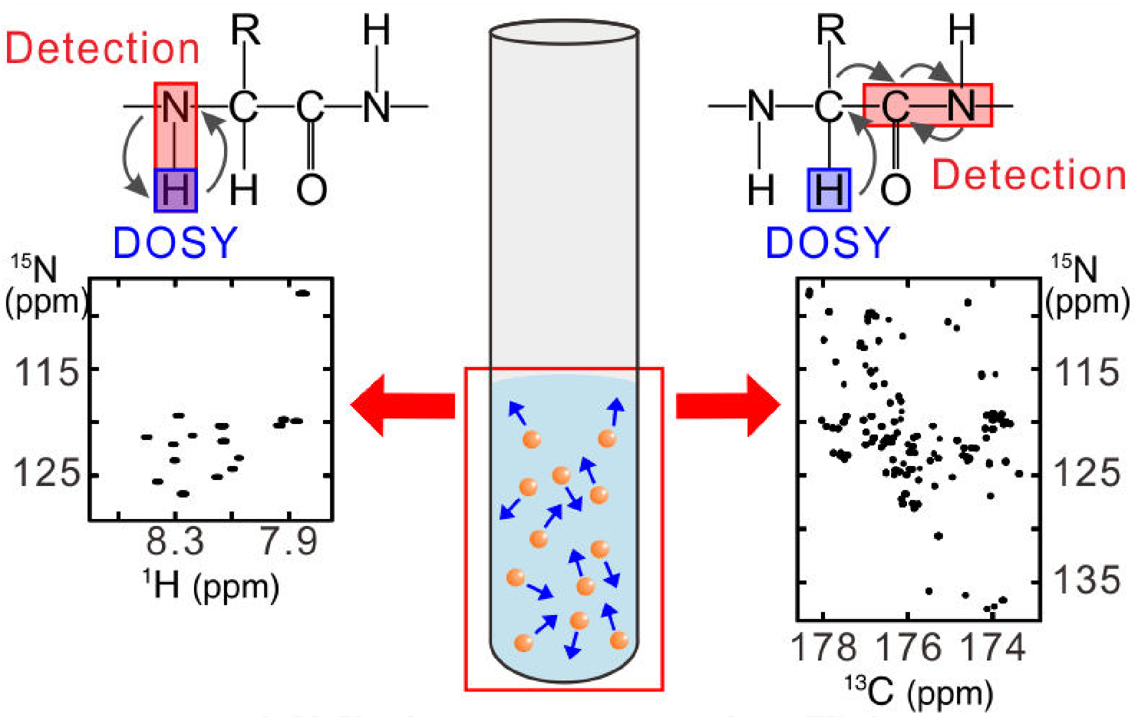
Exhibition Hall C THU 11:00~13:00

Development of a high-resolution NMR technique to measure diffusion of proteins at near-physiological conditions

Jongchan Lee, Sho Hee Park, Jung Ho Lee*

Division of Chemistry, Seoul National University, Korea

Measuring the translational diffusion of proteins can provide useful information about their size, shape, and surrounding environments. NMR technique, called diffusion NMR or diffusion-ordered spectroscopy (DOSY), is widely used to study the diffusion of molecules, mainly observed using protons since they have a high gyromagnetic ratio. To acquire additional resolution, multidimensional DOSY spectra can be recorded by utilizing the proton-attached heteronuclei. For example, high resolution can be obtained by the combination of the backbone amide protons to measure diffusion with the well-resolved $^{1}H/^{15}N$ correlations. However, at physiological temperature and pH conditions, amide-water proton exchange occurs very quickly, which may reduce the accuracy of diffusion data or lead to complete loss of the DOSY signals. Although diffusion can be measured using aliphatic protons that do not exchange with water protons to overcome such drawbacks, recording the $^{1}H/^{13}C$ correlations often causes spectral overlap, or is obscured by a huge water signal. In this study, we have proposed a method that separates the nuclei used for diffusion measurement (alpha protons, $^{1}H^{\alpha}$) and those used for detection ($^{1}H/^{15}N$ and $^{13}C'/^{15}N$ correlations). This effort improved the resolution of diffusion measurements on polypeptides in a mixture of biomolecules, thereby permitting the investigation of coexisting species under near-physiological conditions


Detection
R
H
N
C
C
N
H
H
O
DOSY
^{15}N (ppm)
115
125
8.3
7.9
^{1}H (ppm)
R
H
N
C
C
N
H
H
O
Detection
DOSY
^{15}N (ppm)
115
125
135
178
176
174
^{13}C (ppm)

Poster Presentation : **PHYS.P-230**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Probing Electronic Structure and Cationic Properties of 2,4-Difluoropyridine: Insights from High-Resolution VUV-MATI Spectroscopy and Quantum Chemical Analysis

Hyojung Kim, Sung Man Park, Chan Ho Kwon*

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

This research delves into the intriguing realm of electronic structure and cationic properties of 2,4-difluoropyridine (2,4-DFP). The substitution of hydrogen with halogen atoms in pyridine has long captured the attention of physical chemists due to its effects on the energy ordering of valence orbitals. This study builds upon prior investigations involving fluoropyridines and difluoropyridines, revealing the intricate interplay of nitrogen-fluorine interactions in altering the highest occupied molecular orbital (HOMO) stability. Leveraging high-resolution vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) mass spectroscopy, we have measured the cationic vibrational spectrum of 2,4-DFP. Analysis of the origin band in the VUV-MATI spectrum has unveiled the adiabatic ionization energy of 2,4-DFP to be 9.9831 ± 0.0004 eV. To gain deeper insights, quantum chemical calculations are employed to scrutinize the measured VUV-MATI spectra. This theoretical exploration promises a comprehensive understanding of the HOMO and cationic structure of the molecule. By synergizing experimental observations with computational analysis, we aim to uncover the intricate relationship between halogen substitution, molecular orbitals, and cationic attributes within the context of 2,4-DFP. This multidisciplinary approach contributes to our broader comprehension of this captivating area of research, with implications for the broader field of physical chemistry and molecular spectroscopy.

Poster Presentation : **PHYS.P-231**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

New source design for laser-desorbed anion formation: Elucidation of the dipole-bound state of diatomic alkali halide anions

Dabin Kim, Sang Kyu Kim*, Sejun An

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

New source design for laser-desorbed anions enables the study of dipolar alkaline halide anions in the gas phase. The combination of laser desorption and filament ionizer is a unique and compact anion source. It is attached to a cryogenic quadrupole ion trap (QIT) and photoelectron velocity-map imaging (VMI) apparatus. The laser desorption is performed with a 532 nm wavelength. After the laser beam is irradiated on the sample disk surface, the vaporized neutrals are delivered into the filament ionizer. By attaching the secondary electron from the filament, the salt complex anions are formed.The QIT enables ions to be trapped and cryogenic-cooled and the trapped ions are transferred into VMI spectrometer. The ions interact with the ns/ps/fs laser beam, and the photoelectron signal is obtained through an MCP detector. Diatomic alkaline halide molecules, such as NaCl and NaI have enough dipole moments over 9 D so that their anions have a dipole-bound state (DBS). The DBS anions have been viewed as the "doorway" of electron attachment processes. In the study of these anions, its characteristic of having only one vibrational mode can provide clear spectroscopic information for DBS studies.

Poster Presentation : **PHYS.P-232**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Parasite exciton dynamics of phosphorescent OLEDs under external bias voltage by time-resolved photoluminescence spectra measurement

HyunJae Lee, Chul Hoon Kim*, Changmin Lee[1], Seung Yoon[1,*]

Department of Advanced Materials Chemistry, Korea University, Korea

[1]*Korea University Sejong Campus, Korea*

We have investigated exciton recombination dynamics of blue phosphorescent organic light-emitting diodes (Ph-OLEDs) through In-situ/operando transient measurements. Time-resolved photoluminescence (TRPL) spectra measurements of the electrically pumped Ph-OLEDs allow us to analyze the exciton recombination dynamics between photo-induced charge carries and electrically supplied ones. We prepared Ph-OLEDs devices with varying the thickness of emissive layer (EML) and deeply studied the variation of recombination zone (RZ) in them via decay-associated spectral analysis of the TRPL spectra. The operando study revealed that the contribution of the parasite excitons on the OLED emission are varied with the EML thickness and the superior efficiency along with optimum color purity are attained with the EML thickness of 15~20 nm.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-233**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Tracking the tunneling potential of photodissociation reaction in methylamine-d2 via IR+UV double resonance spectroscopy

Minseok Kang, Sang Kyu Kim*

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

Methylamine shows a N-H(D) bond fission photodissociation reaction through the tunneling whose barrier is generated by avoided-crossing with the upper state (S2(nσ^*)) in S1(3s←n) state. Interestingly, the tunneling coordinate (correlated with N-D stretching vibration) is strongly coupled with the torsion vibration of the methyl rotor. The methyl rotation is a near free rotor (~5 cm-1) in the equilibrium structure of the S1 state, and can be simulated through free rotor Hamiltonian combination with overall rotation, which is consistent with the experimental results of resonant two-photon ionization (R2PI) experiment.Here, we identified a high quantum number state of internal rotor (m > 8) that did not appear in the R2PI spectrum using the IR-UV double resonance spectroscopy. It confirmed that these rotor states reflect the potential of tunneling reaction as a large-amplitude motion. Using an IR laser, pre-excitation was performed to a specific ro-vibration state of the molecule, and the rovibronic structure in the S1 state was obtained through UV laser. Interestingly, super rotor states of m > 8 could be observed (previous R2PI spectrum observed up to the m=4 quanta), and their energy is negatively deviated from the energy predicted in the free rotor model, which means that the wavepacket exists the somewhat elongated N-D bond length. Based on these experimental findings, the shape of the tunneling potential could be expected by tracking the energy of the super rotor state. Also, ab initio calculation was also consistent with experimental results.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-234**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Ultrafast study of the photodissociation for iodo-phenolate anions in solution with UV pump

Chanho Park, Sang Kyu Kim[*]

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

Phenolate anion is a part of tyrosine amino acid, and it is commonly found in the bioactive chromophores such as the photoactive yellow protein (PYP) and the green fluorescent protein (GFP). In the solution phase, the phenolate anion undergoes photo-oxidation process with UV excitation. Introducing the halogen atom to phenolate anion could provide a heterolytic C-X bond dissociation channel, which is absent in the bare phenol. However, the excited state dynamics of halo-phenolates have been dealt with nanosecond laser system.In this presentation, the excited state dynamics of iodo-phenolate (IP-) anions dissolved in solution was investigated through femtosecond transient absorption (TA) spectroscopy. Upon UV (300~310 nm) pump excitation, the cleavage of C-I bond is preferred to photo-oxidation process for all three mono-iodine substituted species, 2-IP-, 3-IP-, and 4-IP-. The absorption of solvated electron signal is barely observed. Excited state absorption of IP- decays with ~150 fs and another relaxation feature, which is probe-wavelength dependent, with several picosecond lifetimes is commonly observed. Interestingly, the second relaxation lifetime of 4-IP- is 2~3 times longer than those of other IP-s. We assume that the second component is originated from the relaxation of photo-products from the comparison between other series of phenolate anions.

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

The synthesis of chiral plasmonic nanoparticles based on understanding of chiral transfer mechanism

Chaeyoung Im, Seunghoon Lee*

Department of Chemical Engineering (BK21 FOUR Graduate Program), Dong-A University, Korea

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 sources such as chiral molecules or circular polarization to effect chiral transfer from achiral to chiral states. Characterization techniques such as Circular Dichroism (CD) and Scanning Electron Microscopy (SEM) were utilized to confirm the property of chiral transfer and further studied what mechanism was chiral transfer. In this study, we systematically investigate the mechanism of chiral 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-236**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Vertical and In-plane $MoSe_2$-WSe_2 Heterostructures Uniformly Grown by Chemical Vapor Deposition Using Liquid Precursors

JooHyeon Ahn, Youngdong Yoo[1,*]

Department of Energy System Research, Ajou University, Korea

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

Heterostructures of transition metal dichalcogenides (TMDCs) exhibit novel electronic and optoelectronic properties depending on their various band structure. Due to their interesting electronic and optoelectronic properties, p-n junction heterostructures of TMDCs have been used for advanced 2D electronics and optoelectronics such as 2D photodetectors and photovoltaic devices. In particular, p-n junction heterostructures with type-II band alignment exhibit rectifying behavior and self-powered photodetection. However, synthesis of uniform p-n junction heterostructures is challenging. Here, we report the synthesis of uniform $MoSe_2$-WSe_2 heterostructures by chemical vapor deposition method using liquid precursors. Interestingly, lateral and vertical junctions coexist in a heterostructure. Over the large area of the substrate, monolayer $MoSe_2$ is synthesized first, and monolayer WSe_2 grow subsequently at the edge of the $MoSe_2$ and on the basal plane of the $MoSe_2$. As-synthesized $MoSe_2$-WSe_2 heterostructures are characterized by various techniques such as optical microscopy (OM), atomic force microscopy (AFM), Raman and photoluminescence (PL) spectroscopy, and scanning transmission electron microscopy (STEM).

Poster Presentation : **PHYS.P-237**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Charge Carrier Dynamics in $CsPbBr_3$ Perovskite Quantum Dots and Nanowires: Insights from FP-TRMC and TCSPC

Bobae Lee, Jaehong Park[1,*]

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

In this study, we investigate the charge carrier dynamics in $CsPbBr_3$ perovskite quantum dots (PeQDs) and nanowires (PeNWs), utilizing flash-photolysis time-resolved microwave conductivity (FP-TRMC) experiment as well as time-resolved photoluminescence (TRPL) spectroscopy. $CsPbBr_3$ PeQDs and PeNWs that were synthesized via a modified hot injection method, exhibit distinct photophysical properties such as complex dielectric response as well as charge-recombination dynamics via FP-TRMC experiments. Our results suggest that the observed differences in carrier mobility can be attributed to the quantum confinement effect coupled with the role of grain boundaries. Additionally, TRPL experiments elucidated the mechanism of charge recombination, providing a comprehensive understanding of the charge dynamics in the investigated nanostructures. The findings from this study offer valuable insights into the design and optimization of perovskite-based devices by leveraging the unique properties, depending on dimensionality in PeQDs and PeNWs.

Poster Presentation : **PHYS.P-238**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis and Characterization of High-Entropy Oxide Cathode Materials with Spinel Structure forHigh-Voltage Lithium-Ion Batteries

Geonhee Kim, **Sanghun Lee**[1,*]

Department of chemistry, Gachon University Global Campus, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

As the demand for lithium batteries in the field of electric vehicles rapidly increases, it is highly required that the battery performance is accordingly advanced. Research for this mission is underway to secure the high voltage, high capacity, and high stability. As one of the candidates for high potential materials, LiMn2O4 with spinel structure has been targeted for long time. Although it possesses a relatively low capacity compared to materials with layered structures, it has advantages of superior voltage and stability. However, the structural stability of LiMn2O4 decreases by the Jahn-Teller effect with atomic transitions occurring during the charge-discharge cycles. To enhance the structural stability of LiMn2O4, we present a spinel-structured high-entropy oxide (HEO) of Li(CrFeMnNiCu)2O4. It has been synthesized by the co-precipitation method, and the structural characteristics has been studied with X-ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP-OES), and energy-dispersive X-ray spectroscopy (EDS). The electrochemical performance has been evaluated by a half coin cell test. The high entropy oxide with a high voltage window which has been successfully synthesized by various metal atoms would be an innovative cathode material with enhanced electrochemical performance for sustainable energy storage systems.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Computational study on the geometric and electronic structures of MoS_2 grain boundaries

Prihatno Fajar, Jaehoon Jung[*]

Department of Chemistry, University of Ulsan, Korea

The growth of monolayer molybdenum disulfide (MoS_2) may lead to a variety of grain boundaries (GBs) due to the different orientations of MoS_2 island. The high-resolution TEM measurement recently presented the appearance of GB in basal plane of monolayer MoS_2, which is composed of tetra-, penta-, and heptagonal geometries and can be emerged due to the different orientation of 18° between two MoS_2 islands.[1] The periodic density functional theory calculations were carried out to understand the stability and electronic properties of observed GB compared with previously theoretically and experimentally reported GBs.[2] In addition, we analyzed the detailed electronic structures of every single polygonal structure, i.e., orbital splitting of Mo atom caused by surrounding S atoms. The unique geometries inside of polygonal structure in observed GB MoS_2 can be categorized with capped trigonal prismatic, tetragonal pyramid, trigonal Mo bond, deficiency of S bond, and Chinese lantern geometries. We further investigated electrocatalytic activity for hydrogen evolution reaction of various GBs MoS_2.1. Ahn, C.; Park, Y.; Shin, S.; Ahn, J.-G.; Song, I.; An, Y.; Jung, J.; Kim, C. S.; Kim, J. H.; Bang, J.; Kim, D.; Baik, J.; Lim, H., ACS Appl Mater. Interfaces 2021, 13, 6805-6812.2.Gao, N.; Guo, Y.; Zhou, S.; Bai, Y.; Zhao, J., J. Phys. Chem. C 2017, 121, 12261-12269.Keywords: MoS_2, grain boundary, hydrogen evolution reaction

Poster Presentation : **PHYS.P-240**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Accelerating Excimer Formation through Dense Assembly of Coumarin Dyes on TiO2 Films

Hyunseok Lee, HyungJoo Lee, Chul Hoon Kim*

Department of Advanced Materials Chemistry, Korea University, Korea

Previously, we reported on the ultrafast dynamics of coumarin (7-hydroxycoumarin-3-carboxylic acid, OHCCA) anchored on ZrO2 and TiO2 films. That study revealed that when dyes anchored on TiO2 films aggregate, excitons form, which can significantly compete with the interfacial charge injection process, potentially reducing the efficiency of semiconductor devices like DSSCs. However, it's essential to determine whether vibrational modes with large nuclear displacements in the excited state play a crucial role as reaction coordinates in the acceleration of exciton formation due to structural reorganizations. Therefore, by using BPHA (2-(4-butoxyphenyl)-Nhydroxyacetamide) as an adsorption pretreatment agent, we aim to induce a higher density assembly of the dye on the TiO2 film, promoting exciton formation, enabling us to observe vibrational modes in the femtosecond domain. We also intend to explore new dynamics using another coumarin (7-(Diethylamino)coumarin-3-carboxylic acid), similar to OHCCA.

Poster Presentation : **PHYS.P-241**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Detection of benzenediol compounds with SERS using Metal-Chelation Nanoshell(MCNS)

Mingyeong Kim, Dae Hong Jeong[1,*]

College of Education Department of Science Education Chemistry Major, Seoul National University, Korea

[1]*Department of Chemical Education, Seoul National University, Korea*

Surface-enhanced Raman Spectroscopy(SERS) is outstanding spectroscopic analytical technology that shows high sensitivity and specificity. However, detection of molecules with SERS mostly depends on interaction between metal and analyte molecules. Thus, detecting molecules such as non-thiol compounds which lacks attractive interaction with the metal in aqueous solution is challenging so far. In this research, we utilized Metal-Chelation to detect benzenediol compounds, dopamine(DA) and catechol to attract and capture the diol compounds to the surface of AgNS. Poly(vinyl)alcohol(PVA) on silver metal nanoshell(AgNS) are used to link AgNS and metal ion by coordinate bond between hydroxyl groups and metal ions. To effectively detect DA and catechol, we optimized reaction procedure by changing metals (Cu, Zn) and capping agents (2-mercaptoethanol and PVA). We successfully detected dopamine(DA) and catechol in aqueous solution using MCNSs. Stability of those particles are also investigated in DW, MgSO4 buffer. Furthermore, for sensitive and uniform detection of diol compounds, MCNS were conjugated on Si wafer with electrostatic attraction. pH dependence of metal-chelation was also investigated with MCNS substrate.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-242**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Enhanced photocatalytic activity of TiO_2 by Fe incorporation towards simultaneous oxidation of NO and acetaldehyde under visible light

Shufang Zhao, Ji Yujing[1], JICHUANG WU[2], Yebin Choi[1], Hyun Ook Seo[3], Young Dok Kim[1,*]

Department of Chemistry, Sungkyunkwan University, China

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

[2]*Department of Chemistry, Zhengzhou University, China*

[3]*Department of Chemistry and Energy Engineering, Sangmyung University, Korea*

Photocatalytic behavior of Fe-modified TiO_2 photocatalysts were studied for the simultaneous oxidation of NO and acetaldehyde under visible light irradiation. The complex and mutual influential photocatalytic activity was evident, Acetaldehyde tended to enhance NO oxidation in the presence of 0.4 wt% Fe-TiO_2 at the initial stage of the reaction, but later reduced the NO oxidation activity. depending on reactants concentrations and photocatalysts structures. Bare TiO_2 showed high selectivity towards NO oxidation. Such complexity in mutual interactions between different pollutants on the photocatalyst surface is a crucial factor, which should be considered in real-world application of photocatalysts.

Poster Presentation : **PHYS.P-243**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Plasmon-Enhanced Hybrid Nanoparticles for Efficient Plastic Degradation

Jeongmin Seo, Seunghoon Lee[1,*]

Chemical Engineering, Dong-A University(BK21 FOUR Graduate Program), Korea

[1] Department of Chemical Engineering (BK21 FOUR Graduate Program), Dong-A University, Korea

This study develops assembled plasmonic metal hybrid nanoparticles that can effectively utilize solar energy to proceed with plastic degradation. We aim to study the plastic decomposition reaction with understanding of the photocatalytic mechanism in photocatalytic reaction. The efficiency of the photocatalytic reaction strongly depends on the morphology and composition of metal nanoparticles. Here we control these parameters to find optimal photocatalytic performance. The synthesized plasmonic metal hybrid nanostructures, Au@Pd nanoparticle clusters(Au@Pd NPCs), can act as efficient photocatalysts to break down plastic waste into smaller molecules such as carbon dioxide, water, and other compounds. Au@Pd NPCs can efficiently convert light to chemical energy with the formation of active oxygen species. Activated oxygen can react with the plastic to break the C-C bonds. We observe the plastic degradation through Dynamic Light Scattering (DLS) analysis of plastic solutions and Scanning electron microscopy (SEM) images. This work can be used for actual hydrogen production, useful organic molecule synthesis, and plastic decomposition through future commercialization.

Poster Presentation : **PHYS.P-244**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

In-Plane Mixed-Dimensional Heterostructures from Monolayer MoS_2 and Low-dimensional Mo/Te Compounds Synthesized by Te-Flux-Controlled Chemical Vapor Deposition

Hyeonkyeong Kim, **Youngdong Yoo**[1,*]

Energy Systems Research, Ajou University, Korea

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

Mixed-dimensional heterostructures formed by combining 2D van der Waals materials and other dimensional (0D, 1D, and 3D) materials with novel properties have attracted attention in recent years. Here, we report a sequential chemical vapor deposition (CVD) growth method for synthesizing in-plane mixed-dimensional heterostructures consisting of monolayer molybdenum disulfide (MoS_2) and low-dimensional molybdenum/tellurium (Mo/Te) compounds. The composition, dimension, and phase of Mo/Te compounds interfaced with 2D 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. Our work provides a novel Te-flux-controlled CVD strategy to construct in-plane mixed-dimensional heterostructures and opens the possibility of edge-contacted mixed-dimensional electronic and optoelectronic applications.

Poster Presentation : **PHYS.P-245**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Enhanced photocatalytic behaviors over Pt-modified TiO_2 towards acetaldehyde oxidation under visible light irradiation: Effect of Pt single atoms dopants

Ji Yujing, Shufang Zhao[1], Yebin Choi, Jichuang Wu[2], Hyun Ook Seo[3], Young Dok Kim[4,*]

Chemistry, Sungkyunkwan University, Korea
[1] *chemistry, Sungkyunkwan University, Korea*
[2] *Chemistry, Zhengzhou University, China*
[3] *Department of Chemistry and Energy Engineering, Sangmyung University, Korea*
[4] *Department of Chemistry, Sungkyunkwan University, Korea*

In this work, we introduce TiO_2 by Pt incorporation for the photocatalytic oxidation of acetaldehyde under visible light irradiation with various humid conditions (0, 30, 60% RH). We highlighted that by controlling the amount of noble metal like Pt as additive to TiO_2 to yield highly dispersed reactive single atoms species, and annealing temperature to alter the coordination structure of the noble metal single atom, one can find the photocatalyst structure with the highest photocatalytic activity for environmental remediation. For real application, Pt-TiO_2 with 0.096 wt% of Pt and annealed at 130 ^oC would be the best choice since it shows a fairly high activity over a broad range of humidity.

Poster Presentation : **PHYS.P-246**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

The Diffusion of Membrane Molecules in small Phospholipid Vesicles: Insights from Molecular Dynamics Simulations

Jaeheon Yang, Bong June Sung*

Department of Chemistry, Sogang University, Korea

The diffusion of bilayer components such as cholesterol and lipids is critical to understanding cellular processes such as cell signaling. The small unilamellar vesicles(SUVs), of which diameter is about 20nm, have drawn attention due to their applicability for drug delivery. While the curvature of most cells and giant unilamellar vesicles(GUVs) may be negligible, the effects of the curvature on the diffusion and the structure in SUVs may be significant. Even though the diffusion mechanism of flat 2D membranes is extensively studied, the influence of curvature on the diffusion mechanism remains unclear. In this study, we conduct molecular dynamics simulations for both 20 nm-sized SUVs with severe curvature and flat 2D bilayer, composed of saturated lipids and cholesterol of cholesterol mole fractions from 0 to 0.5. We find that cholesterol concentration is higher in the inner leaflet. Our results also show that the diffusion of lipids in SUVs is up to 2 times faster than in 2D membranes. Moreover, the diffusivity in the outer leaflet of SUVs is higher than that in the inner leaflet.

Poster Presentation : **PHYS.P-247**

Physical Chemistry

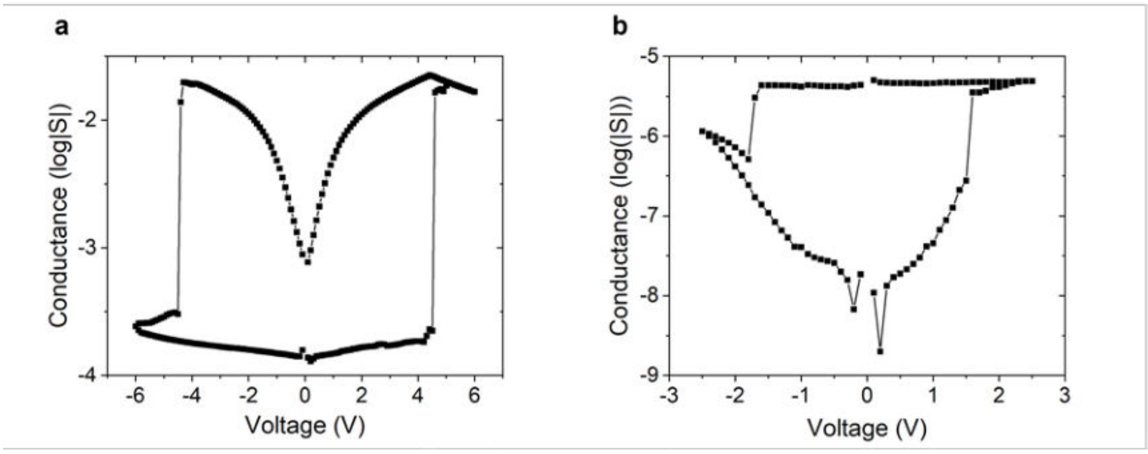
Exhibition Hall C THU 11:00~13:00

Anisotropic charge transport in memristive behavior of MXene

Suji Ha, Junwoo Park*

Department of Chemistry, Sogang University, Korea

2D Titanium carbide (Ti_3C_2) MXenes possess both high conductivity and a large surface area with hydrophilic functional groups. Their good dispersibility makes MXenes suitable for cost-effective, large-scale solution processing. As a result, MXenes have attracted widespread attention across a variety of applications, such as chemical sensing, electromagnetic interference shielding, energy storage systems, and electronics.In this study, we investigate distinct anisotropic electrical transport in metallic Ti_3C_2 MXene films with EGaIn liquid metal electrodes, depending on the electrode configuration (vertical and horizontal). The low-resistance state in the vertical configuration exhibits ohmic behavior (Figure a), while the ohmic behavior is observed in the high-resistance state in the horizontal configuration (Figure b). This result suggests that the conduction mechanisms in the two different configurations have entirely different characteristics, accompanied by conductance hysteresis.We assumed that the direction of charge flow (i.e., in-plane and out-of-plane) creates differences in the conduction mechanism, leading to conductance hysteresis. Not only the direction of charge flow but also the MXene-EGaIn interface will be a primary reason for this hysteresis. This work will contribute to (1) understanding the anisotropic charge transport of MXenes and (2) suggesting potential applications of MXenes as candidates for memristors in neuromorphic computing.


a
Conductance (log|S|)
-2
-3
-4
-6
-4
-2
0
2
4
6
Voltage (V)
b
Conductance (log(|S|))
-5
-6
-7
-8
-9
-3
-2
-1
0
1
2
3
Voltage (V)

Poster Presentation : **PHYS.P-248**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

The Role of Soft Segments on the Stress Relaxation of Thermoplastic Elastomers

Hyungshick Park, Bong June Sung[*]

Department of Chemistry, Sogang University, Korea

Although thermoplastic elastomers (TPEs) have been used commercially since the 1950s, there is a still lack of understanding about their molecular level mechanism on stress relaxation. TPEs are block copolymer with hard (crystallizable) and soft polymers. Hard segments (HSs) form crystallized domain, while soft segments (SSs) are still amorphous and mobile at room temperature. Previous studies suggested that crystalline domains and entanglement of SSs cooperatively act as topological links. And these topological links are key to understand the mechanical properties of TPEs. However, it is hard to understand these network structures because of the anisotropic nature of crystallites. In this work, we investigate the structural changes of HS and SS during deformation. And we investigate the contribution of each segment to their mechanical properties. We find that Young's modulus decreases with increasing length of SSs. To understand the role of each segment, we calculate the contribution of hard and soft segments to the total stress. We find that the stress contribution of hard segments decreases with increasing soft segments. We conclude that SSs relax the applied stress and also reduce the applied stress to the crystallites. As a result, the alignment of crystallites and the decrease of crystallinity are reduced with longer SSs. We also analyze averaged length between crystallites and entanglement length of SSs to understand the role of SSs during deformation. We find that SSs connect crystallites in long-range compare to the average distance between crystallites. In addition, we analyze the number entanglement of kinks during deformation and find that SSs rapidly relax the stress and the number of kinks is constant.

Poster Presentation : **PHYS.P-249**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Ultranarrow Quantum Plasmon Resonance of Self-doped Ag2Se Nanocrystal in Mid-Infrared Region

Haemin Song, Jin Hyeok Lee, So Young Eom, Dongsun Choi, Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

The quantum plasmon resonance (QPR) exhibits the combined properties of classical and quantum mechanics, which could lead to the new physical, optical features. However, research on the QPR has been limited owing to the difficulties of increasing the carrier density of semiconductor nanocrystals (NCs). Herein, we present the QPR of a self-doped Ag2Se NC in mid-infrared region with an extremely narrow bandwidth. As the size of the NCs become large by passivating the NC surface with chloride ligand, the Ag2Se NCs can be highly self-doped due to the weakened quantum confinement effect. The QPR feature was thoroughly investigated by infrared spectroscopy, ultraviolet photoelectron spectroscopy, and the photoluminescence spectroscopy. Two theoretical models that combined the characteristics of the metal and semiconductor were used for the analysis, which revealed the QPR coupling with the intraband transition and the limited nature of electron density in semiconductor NCs. The effect of the quantum confined plasmon resonance reduces the peak bandwidth to 19.7 meV, which indicates 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.

Poster Presentation : **PHYS.P-250**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

The modeled protein structure quality assessment via Graph neural network

Jinyoung Byun, Juyong Byun[1,*]

college of pharmacy, College of pharmacy Seoul National University, Korea

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

Proteins play a pivotal role in biological processes, often interacting to form complexes that execute essential functions. The accurate prediction and assessment of the quaternary structures of these protein complexes remain a significant challenge, especially in estimating the quality of predicted structures without reference to native configurations. Recent computational advancements, based on AlphaFold-multimer, have made strides in this domain. However, one of the importanthurdles which makes users confused is what is the real structure. and which structure is more reasonable? Traditional methods like convolutional neural networks (CNNs) are proposed for this problem but are not rotation invariant, necessitating data augmentation that can hinder computational performance. To address this, we introduce graph neural networks (GNN) based for assessing a modeled protein structure. By representing protein or protein-protein complexes as rotation-invariant graphs, we leverage the capabilities of GNNs, bypassing the limitations of CNNs. Additionally, to overcome the limitations of the number of data, which is one of the main issues in this domain, we use the AlphaFold human database structure which have domain information from Uniprot. This integrated approach not only offers a robust solution for protein structure model quality assessment but also holds promise for applications in drug discovery, protein engineering, and function analysis. Furthermore, we expect that the application of transfer learning enhances performance in specific downstream tasks.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-251**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Charge-carrier dynamics in Organic Photovoltaic Materials

Na Won Park

Ewha Womans University, Korea

The microscopic electron-donor (D) and acceptor (A) domains and their blend interfaces are the main sites for free-charge generation and transport. Therefore, the molecular packing and nanoscale morphology of the active layer play an important role for a device performance in organic optoelectronics including photovoltaics. We utilized flash-photolysis time-resolved microwave conductivity (FP-TRMC) experiments to explore Charge-carrier dynamics in Organic Photovoltaic Materials. FP-TRMC is an electrodeless photoconductivity measurement which can figure out carrier information like carrier generation yield (ϕ), mobilities ($\sum \mu = \mu e + \mu h$, the sum of electron/hole mobilities), and recombination dynamics. We compared charge-carrier dynamics of PM6: non-fullerene acceptor blend with several additives. We confirmed that the presence of MXene in the photoactive layer leads to improving free-charge generation by facilitating polaron pair dissociation. Also, we figured out that using 2PACz as an additive in PM6:Y6 blend gives longer carrier lifetime.

Poster Presentation : **PHYS.P-252**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Excimer Formation in Polycrystalline PBI Films: Dependence on Packing Geometry

Seongsoo Kang, Dongho Kim[1,*]

Yonsei University, Korea

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

This study investigates how packing geometries influence excited-state dynamics in films of perylene bisimides (PBIs). The molecular structure of PBIs was modified to control how they are packed in the solid state, and PBI films were fabricated on SiO2 substrates using the physically evaporated deposition method. Three films of each PBI exhibited distinct steady-state absorption and emission spectra. Excimer-like states were observed in PBI1 and PBI2, with the degree of excimer formation dependent on the orientation and packing of PBI molecules within the film. Interestingly, PBI2 showed minimal changes in absorption spectra, except for a slight redshift and spectral broadening, compared to the monomer's steady-state absorption spectra. Femtosecond transient absorption spectroscopy measurements confirmed this peculiarity. We suggest that thermal motion and intermolecular interactions can overcome the steric hindrance of PBI2 molecules, causing structural changes in the excited state. This study provides a better understanding of how crystalline order impacts excited-state dynamics and the formation of the excimer-like state.

Poster Presentation : **PHYS.P-253**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Excited-state dynamics of cobalt-based photocatalyst using X-ray and optical transient absorption spectroscopies

Seung Yeon Choi, Tae Kyu Kim[1], Tae Wu Kim*

Department of Chemistry, Mokpo National University, Korea

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

Transition metal complexes (TMCs) have gained increasing attention because of their versatile functions in solar energy conversion and photonic applications arising from inter-metal or metal-ligand electronic coupling. Excited-state potential energy surfaces and electronic behaviors in TMCs are directly associated to the rate of photo-induced charge transfer, which is one of the key factors to regulate macroscopic photocatalytic activities. To investigate the ultrafast electronic dynamics of metal-based photocatalyst, femtosecond X-ray spectroscopies have been developed by using the X-ray pulse generated from X-ray free electron laser (XFEL), instead of optical pulse, as a probe. X-ray probing pulse can provide the chemical information about the local electronic and nuclear structures of the metal-centers due to superb elemental specificity and thus it is a complementary method to femtosecond optical spectroscopy. In this study, we investigated the photo-induced ligand-to-metal charge transfer (LMCT) dynamics in the cobalt-based complex by employing the femtosecond X-ray transient absorption (XTA) and optical transient absorption (OTA) spectroscopies. The results show that the intersystem crossing pathway was formed through the occurrence of LMCT dynamics in the ultrafast time region. This study will enable us to map out the electronic configuration in the metal-centered 3d orbital, which is a key factor for the photoinduced charge transfer between the ligand and metal moieties.

Poster Presentation : **PHYS.P-254**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigating binding affinities of coomasive brilliant blue in protein-dye complex; Structural insight from the theoretical calculations of X-ray scattering data

Junu Bae, Tae Wu Kim*

Department of Chemistry, Mokpo National University, Korea

The recent study in the field of cell biology reported that a structural analog of coomasive brilliant blue R (CBB-R) acts as a counter partner against ATP-sensitive purinergic receptors, implying the potential application to a pharmaceutical agent. In this study, we focused on investigating the chemical effects of CBB-R dye on the proteins existed in the bloodstream. For hemoglobin (Hb), the interactions between Hb and CBB-R were examined by varying the environmental pH covering from 6.0 to 8.0. We found that the binding constant (Ka) of Hb-dye complex was maximized at the neutral condition and its binding ratio was 1.5. In contrast, the Ka values in acidic and basic conditions were decreased relative to that in the neutral condition. We performed the additional experiments using bovine serum albumin (BSA) protein, which has the simpler structure than that of hemoglobin. The characterization of binding affinity for BSA showed that the Ka value was hugely decreased, while its binding ratio was similar to that in Hb. To understand the structural changes in protein-dye complexes, the degrees of secondary structural change were examined by employing circular dichroism spectroscopy. From this measurement, the larger structural change was observed in the Hb-dye complex compared to that in the BSA-dye. To estimate the protein conformations of the complexes, we performed the theoretical calculations of X-ray solution scattering (XSS) curves based on the modelled structures. This results show that the degree of change in the protein conformation can be accessible in the resolution of XSS. This information from the theoretical study will be utilized for the actual X-ray scattering experiment in near future.

Poster Presentation : **PHYS.P-255**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Structural changes of thioflavin T during intramolecular charge transfer studied by time-resolved vibrational spectroscopy

Sebok Lee, Taehyung Jang, Yoonsoo Pang*

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

Intramolecular charge transfer (ICT) is one of the fundamental chemical reactions, and has been of great interest in chemistry and related fields for many decades. Although the structural changes of push-pull chromophores during the ICT process have been widely estimated in the theoretical investigations by time-dependent density functional theory (TDDFT) and molecular dynamics simulations, the experimental evidence by time-resolved spectroscopic methods has been rarely available. Recently, we showed that the skeletal vibrational modes of ν8a and νC=C modes in the frequency range of 1500-1650 cm-1 obtained from femtosecond stimulated Raman spectroscopy (FSRS) with both high spectral ($^{-1}$) and temporal ($^{-1}$, which is interpreted as the in-plane and out-of-plane deformations of the dimethylaminophenyl and benzothiazole backbone. The ultrafast changes in these vibrational modes provides the experimental evidence for the vibrational relaxations of the Franck-Condon state and the subsequent ICT dynamics. On the other hand, FSRS measurements provide the excited-state Raman spectra of thioflavin T in the ICT state, where only peripheral structural changes such as the twist of electron donor dimethylaminophenyl group can be expected from the blue-shifts of the skelectal νring(C=C) modes. By combining the time-resolved vibrational measurements of thioflavin T in aliphatic alcohol solvents, the detailed structural changes of thioflavin T during the ICT will be sought, which may occurs via separable structural chages including the bend of benzothiazole moiety and the twist of dimethylbenzothiazole group.

Poster Presentation : **PHYS.P-256**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Relativistic Mixed-Reference Spin-Flip (MRSF)-TDDFT

Konstantin Komarov , Cheol Ho Choi[1,*]

Center for Quantum Dynamics, Pohang University of Science and Technology, Russia

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

The development of Relativistic MRSF-TDDFT takes into account spin-orbit coupling (SOC) through a mean-field approximation. This enhanced SOC-MRSF method remarkably aligns with experimental data, and its accuracy is further supported by comparisons with four-component (4c) relativistic CASSCF and 4c-CASPT2 methods, particularly in the calculation of spin-orbit-energy splitting for Carbon, Silicon, and Germanium atoms. Impressively, even for Tin, a fifth-row element, the method estimates splittings with an error margin of approximately 3%. When applied to molecular calculations of 4-thiothymine featuring a third-row element, SOC-MRSF outcomes align closely with those derived from the SO-GMC-QDPT2 level, regardless of the geometry or exchange-correlation functional used. The method also successfully predicts the likelihood of S1 (nπ∗) to T1 (ππ∗) intersystem crossing in thymine, which contains only second-row elements. Given its precision and applicability, SOC-MRSF could be a reliable tool for tackling complex electronic structure challenges, such as nonadiabatic molecular dynamics that include both internal conversions and intersystem crossings in large-scale systems.

Poster Presentation : **PHYS.P-257**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Tracking electronic dynamics of pristine and blue TiO2 nanocomposites under various catalytic conditions

Woo hyeok Kim, Seung Yeon Choi[1], Tae Wu Kim[1,*]

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

Titanium dioxide (TiO2) is an inorganic semiconductor photocatalyst and has been used for the various photocatalytic applications such as artificial photosynthesis or hydrogen evolving reaction due to its excellent catalytic activity and superb chemical stability. [1] 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. [2] Despite the numerous studies, the detailed information about the photo-induced charge carrier dynamics in the B-TiO2 is elusive. 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 experiments based on the real-time tracking manner. Especially, we employed the various chemical conditions such as the uses of acid and hole scavenger in order to study the effect of the environmental condition in the photo-induced electronic dynamics. From the systematic study, it was confirmed that the electron-hole geminate recombination in B-TiO2 was significantly delayed relative to that in the pristine one, which is a key factor to regulate the macroscopic catalytic activity. It was also revealed that the excited-state charge carrier dynamics was hugely affected by the external pH condition and the use of hole scavenger resulted in the prolonged dynamics of trapped electrons, which showed a stark contrast to the dynamics of trapped holes.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-258**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Enhancing the methanol oxidation activity of Pd@Pt by modulating synergistic effects

Hyeon Jeong Kim, Young Wook Lee[1,*]

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

The single-pot production of Pd@Pt core–shell structures is a promising approach as it offers high surface area, catalytic capability, and stability. In this work, we established a single-pot process to produce Pd@Pt core–shell nanodendrites with uniform shape and tunable size and composition for optimal electrocatalytic activity. Pd@Pt nanodendrites with different compositions were synthesized by adjusting the ratios of Pd and Pt precursors in an aqueous environment using cetyltrimethylammonium chloride, which acted as both the surfactant and the reducing agent at an elevated temperature (90 ℃). The synthesized $Pd_5@Pt_5$ nanodendrites showed exceptional electrocatalytic performance toward the methanol oxidation reaction compared with other compositional Pd@Pt nanodendrites and conventional Pt/C electrocatalysts. Their CO tolerance was attributed to surface structure and the synergistic effect between Pt and Pd. Compared to Pt/C, $Pd_5@Pt_5$ nanodendrites exhibited significantly higher anodic peak currents in terms of mass and electrochemical active surface area-normalized current density. This approach offers a promising strategy for designing electrocatalysts with unique structures and superior catalytic performance and stability in electrochemical energy conversion.

Poster Presentation : **PHYS.P-259**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Comparison of HMF to FDCA Conversion Efficiency and Methods for Performance Improvement of BiVO4 Photocatalyst

Myung Jong Kang*, **Serin Jung**

Department of Chemistry, Gangneung-Wonju National University, Korea

As global warming caused by excessive CO2 concentration on atmosphere and plastic crisis, researches on eco-friendly materials are also actively studied. Because 5-hydroxy methylfurfural (HMF), obtained from biomass, can be converted into various value-added chemicals, researches on HMF conversion into value added chemicals studied widely. Among several conversion products, 2,5-furandicarboxylic acid (FDCA) is regarded as green material to replace pristine petroleum derived plastics. FDCA can be combined with ethylene glycol to create an eco-friendly material called polyethylene furanoate (PEF) that can replace polyethylene terephthalate (PET). PEF not only has the advantage of being an eco-friendly material but also it can be decomposed after-used faster than pristine PET, resulting in less environmental contamination.There are two major methods to convert HMF to FDCA, one is the electrical oxidation and the other is aerobic oxidation. Among the two methods, in this study, electrical oxidation of HMF to FDCA is studied intensively. HMF oxidation was carried out using a photoelectrochemical cell (PEC cell), and BiVO4 was used as the photocatalyst, which has an appropriate band gap and little toxicity. To overcome drawback on BiVO4 for practical usage, two different strategies were used to improve possibility of commercialization of photoelectrochemical HMF oxidation reaction with BiVO4 photocatalyst.

Poster Presentation : **PHYS.P-260**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Synthesis Waste Melamine formaldehyde Resin and Metal with Urea, applied into Photocatalytic Electrode

Myung Jong Kang[*], Kyong Suh Kim

Department of Chemistry, Gangneung-Wonju National University, Korea

Melamine formaldehyde resin made by the polymerization of melamine and formaldehyde, widely used in the world such as cookware, dishes and building material because of their good properties of thermal and chemical stability, low cost, and light weight. However, after-used melamine formaldehyde resin causes serious environmental problems called as ‘plastic crisis’ because of it takes about 500 years to decomposed completely in naturally.Graphitic carbon nitride (g-C_3N_4), a kind of photocatalyst, can be synthesized from Melamine, Urea, Dicyandiamide (DCDA) through a high temperature process. g-C_3N_4 have high stability, economic, and characteristic on absorbing visible light to utilize solar light energy. In this reason, we studied about upcycling the waste melamine resin to synthesizing g-C_3N_4 photocatalysts, and adding metal ions on them to improve photocatalytic efficiency of waste melamine formaldehyde resin upcycled g-C_3N_4 photocatalysts. In addition, we studied on method to fabricate photoelectrode to apply waste melamine formaldehyde resin upcycled g-C_3N_4 photocatalyst into photoelectrochemical reaction.

Poster Presentation : **PHYS.P-261**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Intramolecular Charge Transfer Dynamics of Anthraquinone Derivatives in the Confined Environments of Reverse Micelles

Taehyung Jang, Sebok Lee, Yoonsoo Pang[*]

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

Excited-state intramolecular charge transfer (ICT) has been extensively studied experimentally and theoretically due to its applications to solar energy conversion, photovoltaics, fluorescence sensing, etc. We have reported the ultrafast (180 fs) ICT dynamics of 1-aminoanthraquinone (AAQ) by time-resolved Raman spectroscopy. The internal rotation of the amino group was observed by the major vibrational modes of νC-N + δCH (1200-1230 cm-1) and νC=O (1300-1330 cm-1) upon ICT. It has been known that the ICT dynamics of AAQ depends on the intermolecular hydrogen bonding of AAQ with protic solvent molecules. Thus, the local environments such as the reverse micelles (RMs), where a reduced microviscosity of solvent nanopools and reduced intermolecular hydrogen bonding with protic solvents are available, are considered as good model systems for a deeper understanding of the ICT dynamics with the concomitant structural changes of chromophores.In this research, the ICT dynamics of AAQ and 1-methylaminoanthraquinone (MAAQ) will be investigated by time-resolved electronic spectroscopy. Inside the RMs, the ICT of anthraquinone derivatives becomes much slower compared to the bulk due to a strongly increased microviscosity. However, the ICT dynamics of AAQ exhibit smaller differences between inside the RMs and the bulk, compared to other fluorophores with no apparent structural changes upon ICT. This can be understood that strongly decreased intermolecular hydrogen bonding inside the microscopic RMs would facilitate the ICT dynamics of AAQ in the RMs. These results show that the hydrogen bonding with protic solvent molecules and increased microviscosity inside the RMs should be considered together to interpret the micelle size-dependent ICT dynamics of AAQ derivatives in the RMs.

Poster Presentation : **PHYS.P-262**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Photoelectrochemical Performance Analysis of Photocatalytic Electrode MgAl-Layered Double Hydroxide(LDH) by a Manufacturing Method

Myung Jong Kang*, Yeonwoo Kim, Geon Hyeong Park

Department of Chemistry, Gangneung-Wonju National University, Korea

LDH (Layered Double Hydroxide) is a hydrotalcite, an inorganic layered material consisting of charge-balancing interlayer anions with a positive charge associated with anionic clays in a structure similar to that of brucite. The structure consists of a cation layer and an anion layer capable of inter-layer ion exchange. Metal hydroxides and anions are arranged in an alternating fashion, and a variety of metal divalent and trivalent cations are added to allow for a variety of combinations of anions and cations due to the excess amounts of anions, resulting in the formation of LDH nanostructures with freely controlled physicochemical properties of LDH. LDHs are synthesized for use as catalysts, catalytic substrates, host materials for nanocomposites, and the like. In this study, we investigated on optimized method to fabricate LDH photocatalytic electrode. A method to utilize MgAl-LDH as a photocatalytic electrode was investigated using Mg(II) and Al(III) ions during LDH synthesis. MgAl-LDH is deposited on the FTO substrate by spin-coating technology, electrodeposition, and drop-coating to fabricate electrodes. For the fabricated electrode, the structural features of MgAl-LDH were measured by XRD, and the surface and component analysis of MgAl-LDH was carried out by SEM and EDS. The photocatalytic electrochemical properties were evaluated by LSV.

Poster Presentation : **PHYS.P-263**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Theoretical Insights into Active Centers of Electrocatalyst with a Strong Metal-Support Interaction for Cost-Effective Synthesis of Ammonia via Electrochemical Nitrite Reduction Reaction

Talshyn Begildayeva, Theerthagiri Jayaraman, Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

A green and highly selective synthesis of ammonia (NH_3) via electrochemical toxic nitrite reduction reaction (NO_2^-RR) in the neutral electrolyte is a cure for both energy and environmental issues. Electrocatalysts with dual nature such as metal and metal-derived material can boost the efficacy of the composite and push the selectivity parameter up. Here, the dual Pd–, Pt–, Ru–, and Ir–CoPi composites with a strong metal-support interaction were obtained via one-pot pulsed laser ablation in liquids (PLAL) method. Among the designed composites Ir–CoPi afforded overall nearly ~100% Faradaic efficiency (FE), mass balance, and selectivity toward NH_3 at lower potentials and reached the highest NH_3 yield rate of 1123.17 mM h^{-1} g^{-1} with 78.1% of toxic NO_2^- removal with $k_{app} = 0.31$ mM min^{-1} under applied –1.6 V vs. Ag/AgCl potential. In situ experiments combined with theoretical calculations revealed the Ir active centers responsible for this outstanding performance of Ir–CoPi. This study provided new opportunities for large-scale NH_3 production through beneficial eco-friendly electrochemical reduction of toxic NO_2^- pollutants.

Poster Presentation : **PHYS.P-264**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Sensitive Chiral Sensing of Glucose by Surface-Enhanced Raman Spectroscopy

Daedu Lee, Yoonsoo Pang*

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

Chiral sensing of biomolecules has been regarded crucial in fields of pharmaceutics, diagnosis, etc. since most biological and physiological processes arise from specific molecular interactions between chiral biomolecules. Circular dichroism has been adopted for the chirality differentiation of various biosamples, but the applications are often limited due to the required sample concentration. Recently, surface-enhanced Raman scattering (SERS) has attracted enormous attention in chiral discrimination where the enantioselective detection of target biomolecules can be determined from spectral changes in the SERS of reporter molecules, often related to their orientational changes, with much higher sensitivity. However, the molecular-level understanding of the chirality-specific molecular interactions and surface adsorption of chiral biomolecules by SERS is not yet clear. In this study, the chiral detection of L-/D-glucose will be described based on the SERS with the reporter molecules of L-/D-phenylalanine (Phe). The SERS spectral changes of L-/D-Phe were observed only when gluocose with the same charality as Phe was added to the Phe-silver nanoparticle mixture. The strong enhancement of δ(COO–) band at 633 cm^{-1} and disappearance of ν_s(COO–) band at 1372 cm^{-1} were observed with the presence of glucose of a desired chirality while no changes in the phenyl vibrational bands were observed. It is considered that the surface adsorption geometry of the carboxylate (of Phe) changes from a bidentate to a monodentate to the silver nanoparticles with the introduction of glucose with a desired chirality. Intermolecular interactions between glucose and Phe with an about 1:1 molecular ratio between glucose and Phe are suggested as the origin of the enantiomeric discrimination of glucose and similar chiral biomolecules.

Poster Presentation : **PHYS.P-265**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Pulsed laser induced synthesis of nickel sulfoselenide for efficient furfural and water oxidation

Theerthagiri Jayaraman, Yewon Oh, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Modulating the active site is one promising strategy to increase catalytic performance. Herein, we could successfully introduce anion substitution to transition metal chalcogenides (TMCs) via pulsed laser ablation (PLA) technique. Nickel sulfoselenide ($Ni_3Se_{4(1-x)}S_{4x}$), nickel selenide (Ni_3Se_4), nickel sulfide (NiS/Ni_3S_4) were prepared by one-pot facile PLA method for furfural (FOR) and water oxidation (OER) reactions. The synthesized materials were characterized by XRD, Raman, FE-SEM, HR-TEM, and XPS analytical techniques. The activity of these catalysts was evaluated by examining the electrochemical oxygen evolution reaction (OER). Nickel sulfoselenide revealed best activity with low overpotential of 327.4 mV at a constant current density of 10 mA cm^{-2} which indicate the proliferation of active sites. While nickel selenide and nickel sulfide showed overpotential of 348.4 mV and 361 mV, respectively. This work demonstrates facile and advanced strategy in the preparation of sulfur modified TMCs electrocatalysts toward high-performance for OER and FOR.

Poster Presentation : **PHYS.P-266**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigating the Effects of FOXA Proteins on Transcriptional Activity in DNA-FOXA Complexes: A Molecular Dynamics Simulation StudyMinjun Jung and Rakwoo Chang* Department of Applied Chemistry, University of Seoul, Korea

Min Jun Jung, Rakwoo Chang*

Department of Applied Chemistry, University of Seoul, Korea

Abstract : Gene expression, the engine of cellular function, is orchestrated by proteins called transcription factors that specifically interact with DNA sequences to regulate their transcription. One protein that stands out in this regulation is histone H1, which plays a crucial role in maintaining the DNA structure within units called nucleosomes during transcription. Recent studies have brought to light a new function for Forkhead Box A1 (FOXA1), a member of the FOX protein family. This protein can take over the role of histone H1 and change how DNA bends during the transcription process, offering a fresh perspective on how genes are regulated. In our research, we explore these groundbreaking observations further. Using computer simulations, we analyzed various pairings of DNA and proteins, which include DNA combined with FOXA1 and mutaion variant. These simulations allowed us to assess several variables including the Root-Mean-Square Deviation (RMSD), which measures how much the structure differs from a standard form, the Root-Mean-Square Fluctuation (RMSF), bending angle which indicates the variability in individual segments of the complex, points of interaction between DNA and proteins as shown by a contact map, and features related to the curvature of the DNA.References[1]Zheng, G., Lu,X.J. and Olson,W.K. (2009) Web 3DNA–a web server for the analysis, reconstruction, and visualization of three-dimensional nucleic-acid structures. Nucleic Acids Res., 37, W240–W246.[2] Marco Pasi, Krystyna Zakrzewska, John H. Maddocks, Richard Lavery, Analyzing DNA curvature and its impact on the ionic environment: application to molecular dynamics simulations of minicircles, Nucleic Acids Research, Volume 45, Issue 7, 20 April 2017, Pages 4269–4277, [3] ARRUABARRENA-ARISTORENA, Amaia,

et al. FOXA1 mutations reveal distinct chromatin profiles and influence therapeutic response in breast cancer. Cancer cell, 2020, 38.4: 534-550. e9.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-267**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Evaluation of the Corrosion Rate for Ni-containing alloys under LiCl Molten Salt

Hyeok Il Kim, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

In molten salt reactor (MSR), the molten salt serves as a coolant. Because the structural materials of MSR are always exposed to coolant, they must have excellent corrosion resistance to molten salt. Therefore, to evaluate the corrosion rates of Ni-based alloys in molten salt, corrosion tests were conducted for alloy 600, alloy 617, and Hastelloy N at 635 ℃ for 100 h in LiCl molten salt under the glove box of Ar environment. Through the amount of weight loss before and after the corrosion test, the corrosion rate of three Ni-based alloys was calculated. On the basis of the results of corrosion rate, we confirmed that Hastelloy N has better corrosion resistance than the other alloys. Furthermore, the changes in the crystal structure, surface morphology, and elemental content of each alloy due to corrosion in LiCl molten salt were analyzed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-268**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Adsorption structure of benzyl alcohol molecule on Ge(100) surface

Yeonju Lee, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

The adsorption structure of benzyl alcohol on a Ge(100) surface was explored using high-resolution photoemission spectroscopy (HRPES) and density functional theory (DFT) calculations. Upon analysis of the O 1s core-level spectra, we observed that only one peak at 531.0 eV, which is assigned to neutral O atom. In the case of the C 1s core-level spectra, we found two distinct peaks at 284.9 and 284.3 eV. The peak at 284.9 eV corresponds to the carbon atom adjacent to the oxygen atom, while the other peak is attributed to the carbon atoms in the benzene ring. On the basis of DFT calculations, we verified that the on-top dissociation pathway is more favorable than the intradimer row dissociation pathway in terms of the activation barrier and the adsorption energy of the corresponding dissociation structure. As a result, the adsorption of benzyl alcohol on the Ge(100) surface occurred through the dissociation reaction, in agreement with HRPES results.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-269**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Investigation on adsorption structure of 1,3-dithiolane on Ge(100) surface

Su-Ji Choi, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

The adsorption configuration of 1,3-dithiolane on Ge(100) semiconductor surface was investigated using high-resolution photoemission spectroscopy (HRPES) experiments. On the basis of the S 2p core-level spectra, we found two peaks at 164.4 and 162.2 eV, which are associated with the positively charged S and neutral S atoms, respectively. It indicates that one of the two S atoms 1,3-dithiolane is positively charged and the other neutral. As a result, we suggest that the adsorption of 1,3-dithiolane on the Ge(100) surface occurs through the S dative bonding, leading to the dative bonded structure

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-270**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

[Withdrawal] Asymmetric Catalyst Design using Machine Learning with fragment count fingerprints and augmented substructure type descriptors

You Kyoung Chung*, Shinwon Ham[1]

Department of Chemistry, Sungkyunkwan University, Korea

[1]*Departmet of Chemistry, Sungkyunkwan University, Korea*

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-271**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

DFT Calculation for the First One-Electron Transfer in CO2 Activation and Reduction Reaction induced by PVP

Mee Kyung Song

Institute for Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

We carried out DFT calculations to assess the consistency between the theoretically expected and experimentally measured values for the PVP-induced CO2 activation and reduction in activation energy, which was the first one-electron transfer process of the CO2RR that is, the rate-determining step. We used simplified model conditions (CO2 in water; VP:CO2 in water). Although it has inherent limitations in accurately reflecting the experimental results stemming from the considerably more complicated conditions of the multilayer Cu/Cu10Sn3 and Cu/Cu10Sn3/rGO/PVP/Nafion dark cathodes in an electrolyte solution of 0.5 M KHCO3 with CO2, we can explain the role of VP in inducing CO2 activation and lowering the energy of [TS]*, which eventually reduced the activation energy for the first one-electron transfer reaction and subsequently promoted the CO2RR. All calculations have been carried out using Gaussian. Optimized structures, molecular orbitals, and energy profile will be presented and compared with the experiments.

Poster Presentation : **PHYS.P-272**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Circular Dichroism Spectroscopy of Jet-Cooled 6,6’-Dimethyl-2,2’-diaminobiphenyl

Ye yeon Kim, Jiyeon Yun, Nam Joon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

Conformational isomerism is often an overlooked form of chirality. We utilized dual-beam resonant two-photon ionization circular dichroism (R2PICD) spectroscopy to acquire the electronic circular dichroism (CD) spectra of jet-cooled 6,6’-Dimethyl-2,2’-diaminobiphenyl (MAP). These CD values serve as evidence for the chirality of conformational isomers. Additionally, the IR-UV double resonance spectra indicated that (R)-MAP existed as a singular conformation within the jet.

Poster Presentation : **PHYS.P-273**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Fully Self-consistent QM/MM for Solvated Systems

Taehwan Jang, **Hyungjun Kim**[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Recently, a large discrepancy in the band edge alignment of various transition metal-oxides in vacuum and in solution has been issued in developing photocatalysts. The discrepancy stems from that the mutual interaction across the surface of the reactive system is different. To analyze a condensed matter, especially in the liquid phase, the quantum mechanics/molecular mechanics (QM/MM) simulations are generally accepted as a costly efficient, and accurate tool. We propose a seamless modeling of van der Waals (vdW) interaction for the coupling between two subsystems in a polarizable embedding scheme where there is only a non-bond interaction. We define the term of vdW interaction as the sum of the Pauli repulsion and dispersion. The Pauli repulsion interaction is modeled by using the electron density of the QM subsystem since the overlapping amount of charge densities in two subsystems has been reported to be proportional to the Pauli repulsion. The long-range dispersion attraction will be described by using Grimme's D3 parameters to treat the remained contribution of non-bond interaction. Furthermore, the polarization of MM subsystems will be handled by calculating induced point dipole reacting to the external potential; therefore, the incorporation of QM into polarizable MM will be accomplished and able to construct mutually polarizable QM/MM. We will implement this method using DFT-CES developed by our group and demonstrate the chemical behavior in the liquid phase such as hydrogen bonding, and geometry change.

Poster Presentation : **PHYS.P-274**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Transformation of High Entropy Prussian Blue Analogue Derived High Entropy Oxide into Alloy via Pulsed Laser for Ammonia Production

Yewon Oh, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Ammonia synthesis via electrocatalytic nitrite reduction reaction ($NO_2H^{-}RR$) in neutral media has great potential to solve energy and environmental issues. Unlike traditional Haber-Bosch approach which require extreme harsh condition, $NO_2H^{-}RR$ can produce value-added ammonia product using toxic nitrite and wastewater. For real application in industry, the development of high selective and superior activity of catalysts is required. Here, we provide a novel method for synthesis of high entropy alloy (HEA) vial pulsed laser irradiation in liquid method. HEA attract numerous interest due to their excellent electrocatalytic properties based on their high mixing entropy and cocktail effect. Phase composition and microstructural characterization of the synthesized materials were performed using XRD, Raman, FE-SEM, ICP, and XPS analytical techniques, and employed as an electrocatalysts for $NO_2H^{-}RR$. This work offering a rapid and facile way to fabricate HEA materials from PBA analogues which can be efficiently utilized for ammonia synthesis via nitrite reduction.

Poster Presentation : **PHYS.P-275**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Examining the Predominant Phenomenon in Liquid Water under 800 nm Optical Laser : Comparing Optical Kerr Effect and Multiphoton Ionization

Kyung Hwan Kim*, MyeongSik Shin, Minjeong Ki

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

Water, one of the most abundant and versatile material on the planet, has studied intensely due to its anomalous properties. Although pump-probe experiment using optical laser as pump signal and XFEL source X-ray as pump successfully investigated rotational anisotropic signal of water induced by the laser pump, discussion on other possible processes such as multiphoton ionization are poorly done. Thus, herein, we report the pump-probe time-resolved X-ray scattering experiment performed at FXL beamline at PAL-XFEL, varying laser fluence from 3 TW/cm2 to 168.53 TW/cm2. The optical Kerr effect and the multiphoton ionization are assumed as two mainly competing process. We observed that multiphoton ionization is possibly dominating on high laser fluence range considering the intensity of anisotropic signal lost its linearity as laser fluence increases.

Poster Presentation : **PHYS.P-276**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Impact of Contortion on Singlet Fission Mechanism

Eunho Hwang, Hyungjun Kim[*]

Department of Chemistry, Incheon National University, Korea

Singlet fission is a photophysical concept involving the generation of two triplet states from a singlet exciton through various pathways. This can occur through direct, super-exchange, or two-step mechanisms. Numerous organic materials have demonstrated the occurrence of singlet fission, with prior literature identifying perylene bisimide (PBI) dimers as promising candidates for this process.Previous research has shown that planar PBI structures can curve like a bow with the introduction of linking molecules at the ortho positions. Synthetic chemists have introduced two molecules to induce conformational changes: benzene and thiophene. These molecules result in PBI adopting syn-conformation (bent structure) and anti-conformation (twisted structure).For our investigation, we selected four models based on crystal structures, examining both vertical and parallel stacking arrangements. By employing restricted active space spin-flip (RAS-SF), time-dependent density functional theory (TDDFT), and constrained density functional theory (CDFT) calculations, we assessed the rates associated with each model.Following a three-state kinetics model, we observed that the parallel orientation favors a direct two-electron transfer pathway, while the vertically stacked structure promotes a more intricate super-exchange mechanism. In addition, we conducted an exciton decomposition analysis to determine the proportions of local excitation (LE), charge transfer (CT), triplet-triplet state (TT), and others. Our findings highlight the feasible singlet fission mechanism in contorted PBI dimers based on the calculated rates. Moreover, this suggests that contorting chemical structures can be effective strategies to induce singlet fission without heavy chemical functionalizations.

Poster Presentation : **PHYS.P-277**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Direct Identification of Benzene-I Atomic Charge Transfer Complex Structure via Time-Resolved X-ray Solution Scattering

Seoyoung Lee, Kyung Hwan Kim[*]

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

Solvent effects play a crucial role in complex interactions between solvents and molecules during a reaction, influencing the stability of certain intermediate or transient states. In the context of radical alkane halogenation for alkyl halide synthesis, solvent effects have been found to be significant in controlling the selectivity of halogen radicals when reacting with substituted alkanes. Previous studies have demonstrated that the use of benzene and other aromatic hydrocarbons as solvents improves the selectivity of Cl radicals when reacting with tertiary carbons in the photo-chlorination of 2, 3-dimethylbutane. Initially, it was suggested that a η6π-complex forms between the radicals and benzene, but later arguments arose proposing the formation of σ-complexes from these π-complexes. Extensive research has been conducted on benzene-radical complexes based on these two proposals. However, a definitive conclusion has yet to be drawn, and recent DFT calculation studies have indicated the stability of the π-complex. Due to the absence of direct structural evidence from spectroscopic techniques, understanding the structure of the key intermediate that regulates selectivity remains controversial. In this study, we aim to elucidate the structure of the benzene-I atom charge transfer complex using time-resolved X-ray solution scattering.

Poster Presentation : **PHYS.P-278**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Ru-nanoclusters with exfoliated black phosphorus via acoustic levitator proceeded pulsed laser process for robust hydrogen evolution kinetics

Juhyeon Park, Ahreum Min, Cheol Joo Moon, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Catalyst-driven electrochemical water splitting is the most efficient way to produce hydrogen. Here we present a striking activation phenomenon of ruthenium (Ru) nanoclusters in a few-law two-dimensional black phosphorus (BP) sheet leading to a significant increase in electrocatalytic hydrogen evolution reaction (HER) activity. The practical utilization of BP relies on the effectiveness of the ablation technique of stand-alone acoustic levitator traveling pulsed laser irradiation (PLIL) to produce high-quality wrinkled nanosheets and modulated surfaces with charge-transferring Ru-nanoclusters. The laser-assisted exfoliation process for layers and sizes of BP sheets with uniform distribution is understood as acoustically-levitated droplets via in situ Raman spectroscopy. Shifts in the A_{1g}, B^{2}_{g}, and A^{2}_{g} Raman peaks of BP due to exfoliation can be observed. In Ru-anchored BP, Ru provides a suitable d-band center for H-adsorption via Ru-H bonds. The electronegativity of Ru is adjusted by phosphorus, which removes electrons from Ru's nucleus, enhancing Ru's ability to desorb hydrogen. The synergy between the charge carrier mobilization properties of BP and the high-density active sites of Ru improves HER kinetics in KOH medium with an ultra-low overpotential of 84 mV at 10 mA/cm^2. Our results elucidate the role of metal nanoclusters on exfoliated BP surfaces and a coordinated strategy for high-density electrocatalysts for energy conversion.

Poster Presentation : **PHYS.P-279**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

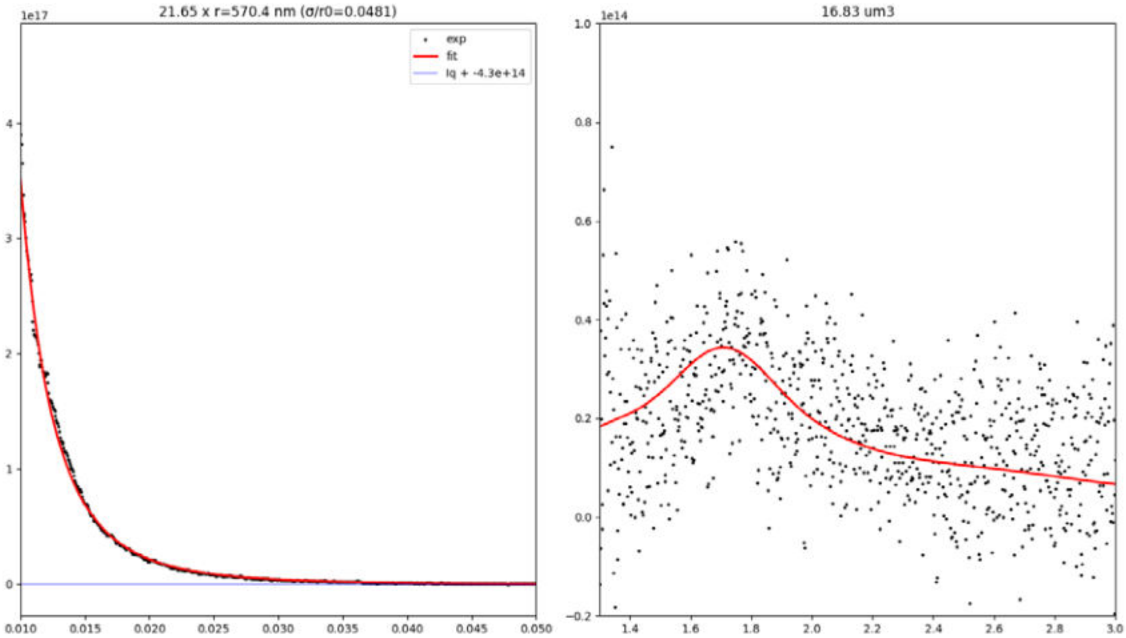
Revealing droplet-size-dependent molecular behaviors in the charged nanodroplets by X-ray scattering

Kyeongmin Nam, Kyung Hwan Kim*, Jongcheol Seo*, Minwook Hwang, Minsu Kim[1]

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

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

Electrospray ionization (ESI) is a method to make a solution sample into gaseous ions by inducing Coulombic explosion of the sample droplets under strong electric field. While the droplets are getting smaller, unique molecular behaviors different from those in bulk solution appear, for example, fast diffusion & mixing in nanodroplets. However, since the nanodroplets are tiny, the detailed mechanism of these intriguing properties are not explored clearly so far. Here, we utilized ultra-short and super-bright X-ray pulse from X-ray free electron laser (XFEL), which enables us to observe samples of molecular-scales. We have developed a custom vacuum-ESI/X-ray scattering chamber to measure wide-angle X-ray scattering (WAXS) and small-angle X-ray scattering (SAXS) to get structural information of Angstrom and sub-micrometer scale (Figure 1). Using this setup, we have been trying to obtain 1) size distribution of the nanodroplets and 2) unique molecular behaviors and their droplet-size dependence like regular assemblies by collecting WAXS and SAXS patterns simultaneously. We have successfully estimated the size of the nanodroplets as shown below (Figure 2) and trying to find clues of the molecular behaviors varying from the size of the nanodroplets.


21.65 x r=570.4 nm (σ/r0=0.0481)
1e17
exp
fit
Iq + -4.3e+14
0
1
2
3
4
0.010
0.015
0.020
0.025
0.030
0.035
0.040
0.045
0.050
16.83 um3
1e14
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-280**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Resolving the fragile-to-strong transition in water by following temperature-induced structural changes and anisotropy

MyeongSik Shin, Kyung Hwan Kim*

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

Most liquids can be classified into two categories, fragile and strong ones, depending on their temperature dependence of the dynamics. Water at ambient temperature and modest supercooled conditions is considered to be a fragile liquid whereas it is proposed to be a strong liquid at temperatures close to the glass transition, which is 135 K. Thus, it is postulated that there exists a fragile to strong transition somewhere in the deeply supercooled regime. By time-resolved X-ray scattering under Optical Kerr Effect (OKE) condition and evaporative cooling in a vacuum can give a chance to find those properties. For the OKE scattering measurement on supercooled water at PAL-XFEL and other XFELs, we have built the equipment that can generate deeply supercooled water droplets and have successfully tested it down to ~227 K. From the recent experiment at SwissFEL, we have measured temperature induced time-dependent structural changes and OKE relaxation of liquid water down to ~228 K.References[1] C.A. Angell, Insights into Phases of Liquid Water from Study of Its Unusual Glass-Forming Properties, Science 2008, 319, 582-587[2] J. A. Sellberg et al., Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature, Nature 2014, 510, 381-384[3] K. H. Kim et al., Anisotropic X-ray Scattering of Transiently Oriented Water, Phys. Rev. Lett. 2020, 125, 076002

Poster Presentation : **PHYS.P-281**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Real-time Tracking of Vesicles in Living Cells Reveals that Tau-hyperphosphorylation Suppresses Unidirectional Transport by Motor Proteins

Donghee Kim, Kyujin Shin[1], Sanggeun Song[2], Mi Hee Lim[3], Ji-Hyun Kim, Jaeyoung Sung[*], Kang Taek Lee[4,*]

Department of Chemistry, Chung-Ang University, Korea
[1]*Hyundai Motor Company, Korea*
[2]*Department of Chemistry, Seoul National University, Korea*
[3]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*
[4]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

Neuronal communication is mediated by the vesicle-transport of motor proteins along the microtubule. Microtubules are destabilized by the hyperphosphorylation of tau proteins; hyper-phosphorylated tau proteins detach from the microtubule and form neurofibril tangles. However, how the phosphorylation of tau affects transport dynamics of motor proteins along the microtubule remains unknown. Here, we report the real-time motion of hundreds of motor protein complexes in living cells under hyperphosphorylation conditions using an upconverting nanoparticle probe. Our investigations reveal that unidirectional motion of vesicle-motor protein multiplexes (VMPMs) is suppressed on the destabilized microtubules, with the consequent loss of fast, long-distance vesicle-transport and that VMPMs suffer partially dynamic motility fluctuations. We establish a parsimonious model of VMPM motion that provides a simultaneous quantitative explanation of various experimental results for VMPM motion in living cells. Our work suggests that the loss of normal vesicle transport along the microtubule is a functional mechanism underlying neurodegenerative disorders associated with hyperphosphorylation of tau.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-282**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Nonadiabatic Molecular Dynamics on the Ultrafast Photoisomerization of 2*H*-1,2-Oxaborine

Sangmin Jeong, Joonghan Kim[1], Kyung Hwan Kim*

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

Photochemistry of benzene has been widely studied including 3 possible photochemical isomers.[1] Employing heteroatoms in benzene cycle, like pyridine and azaborine, has been reported that Dewar form isomer is the main product of the photoisomerization.[2] For azaborine, there has been theoretical investigation with multireference calculations, informing that photoisomerization process occurs through the S_1/S_0 conical intersection.[3] In this work, we modified the heteroatom of the ring from nitrogen to oxygen(2*H*-1,2-oxaborine, denoted as oxaborine), and performed nonadiabatic molecular dynamics simulation of it. From the result of the calculation, the yield of the Dewar isomer is increased, compared to the result of the azaborine. These outcomes are in line with findings from the static potential energy surface calculation result, implying a barrierless decay toward Dewar conformation right after the S_1/S_0 nonadiabatic transition. This result suggests us that the further increase of photoisomerization rate can be achieved toward the O-B functionalization of aromatic molecule.References[1] Bryce-Smith, J. and Gilbert, A.; Tetrahedron 1976, 32, 1309-1326[2] Brough, S. et al.; Angew. Chem. Int. Ed. 2012, 51, 43, 10880-10883[3] Jeong, S. et al.; Phys. Chem. Chem. Phys., 2023, 25, 17230

Poster Presentation : **PHYS.P-283**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

High-entropy alloys (Au, Pt, Pd, Ru and Ir) via CO_2 Laser for Hydrogen Evolution Reaction with seawater splitting

Chae Eun Park, Gyoung Hwa Jeong, Myong Yong Choi[1,*]

department of chemistry, Gyeongsang National University, Korea

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

High Entropy Alloy (HEA) is a new type of single-phase solid solution material with more than 5 metals. High entropy alloys have potentials due to their excellent properties such as thermal stability at high temperatures, and excellent destructive personality at very low temperatures. In this study, HEA (Au, Pt, Pd, Ru and Ir) was synthesized by using CO_2 laser. CO_2 laser have the advantage of being able to synthesize materials in a short time by irradiating high power with thermal energy rather than light energy. Our synthesized HEA materials' characterizations were investigated from SEM, TEM, XRD, XPS and ICP measurements. In addition, the electrochemical test on the hydrogen evolution was performed to measure their catalytic activities. HER were performed in three solutions: 1 M KOH, 0.5 M NaCl, and seawater. HEA-60, the most efficient sample, showed more high activity than the commercial Pt/C in all three solutions.

Poster Presentation : **PHYS.P-284**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Circular Dichroism Spectroscopy of Protonated Phenylalanyl-alanyl-alanine Ions Stored in the Cryogenic Ion Trap

Jinho Jeong, Iltae Yoo, Nam Joon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

Phenylalanine is an alpha amino acid used to synthesize proteins and is a representative chiral molecule used in vivo as precursors such as tyrosine, dopamine, epinephrine and melanin. Alanine is also an amino acid used for protein synthesis and combines with phenylalanine to form various proteins. In this work, we obtained the UV photodissociation (PD) spectrum of protonated phenylalanyl-alanyl-alanine (H+Phe-Ala-Ala) ions produced by electrospray ionization and stored in a cryogenic ion trap near the origin band of the S0-S1 transition. In order to check the number of conformers, the IR ion dip spectra was obtained from 3000 to 3700 cm-1, and at least two conformers were found in the origin band through the IR-UV hole burning spectrum. The structures of the two conformers were identified by comparing the IR ion-dip spectra with the theoretical IR spectra. We obtained the UVPD circular dichroism (CD) spectra of H+Phe-Ala-Ala near the origin bands of the two conformers using the multiple laser shots technique, which showed that the CD values of one conformer was much greater than those of the other. The relationships between the structures of the conformers and their CD values will be discussed.

Poster Presentation : **PHYS.P-285**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

High-entropy Alloys (HEA) and Graphene Oxide (GO) Composites for the development of water splitting system under acidic condition

Yeryeong Lee, Gyoung Hwa Jeong, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Water splitting consists of two reactions, hydrogen evolution and oxygen evolution, and the energy requirements at the cathode and anode vary depending on the pH of the solution. Therefore, hydrogen generation is more efficient under acidic conditions, while oxygen generation is favored in alkaline conditions. We compared these two extremes and a neutral condition to find the optimal reaction conditions, totaling three different scenarios. To achieve this, we employed high-entropy alloys and considered metal alloys to activate hydrogen and oxygen reactions in water splitting. We further synthesized these alloys with graphene to enhance their catalytic performance. As a result, samples synthesized using the pulsed laser irradiation (PLI) demonstrated excellent reactivity in acidic conditions for the hydrogen evolution reaction (HER) and in alkaline conditions for the oxygen evolution reaction (OER). Subsequently, we conducted water splitting experiments under various pH conditions. We confirmed that the reaction was most efficient in KOH alkaline conditions, highlighting the crucial role of OER in water splitting. To further enhance efficiency, we used Pt/C as the standard electrode in acidic conditions and IrO2 in alkaline conditions for measurement. Stability tests also revealed the stability of both the cathode and anode electrodes.

Poster Presentation : **PHYS.P-286**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigating the superheating and melting dynamics of crystalline ice in ps/ns timescale with TRXS

Kichan Park, Kyung Hwan Kim[1,*]

Chemistry Department, Pohang University of Science and Technology, Korea

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

Melting of ice has been investigated intensively for the reason that water is one of the principal substances for lives on Earth. By studies with MD simulations and IR time-resolved spectroscopy, melting dynamics of ice has been studied and several schemes in picosecond and nanosecond time scale were suggested[1, 2]. However there is still intense controversy on timescale ice melting mainly appears. Our group investigated the detailed melting/recrystallization dynamics of crystalline ice (I) especially in nanosecond timescale, with X-ray time-resolved scattering advantageous for more direct structural information[3]. Utilizing the high resolution of XFEL, we are supposed to observe the melting dynamics in earlier time through experiments in this year, and discuss the mechanism of superheating/melting in overall timescale. References[1] Schmeisser, Marcus, Hristo Iglev, and Alfred Laubereau. “Bulk Melting of Ice at the Limit of Superheating.” The Journal of Physical Chemistry B 111, no. 38 (2007): 11271–75.[2] Iglev, H., M. Schmeisser, K. Simeonidis, A. Thaller, and A. Laubereau. “Ultrafast Superheating and Melting of Bulk Ice.” Nature 439, no. 7073 (2006): 183–86.[3] Yang, Cheolhee, et al. “Melting Domain Size and Recrystallization Dynamics of Ice Revealed by Time-Resolved X-Ray Scattering.” Nature Communications 14, no. 1 (2023): 3313(1-7).

Poster Presentation : **PHYS.P-287**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Insights into the Behavior of Chlorosulfolipids and Dipalmitoyl-Glyceryl-Trimethylhomoserine: Coarse-Grained Simulation and Phase Diagram Analysis of Mixed Membrane Systems

Janghee Hong, Rakwoo Chang*

Department of Applied Chemistry, University of Seoul, Korea

This study investigates the behavior of chlorosulfolipids (CSLs) and dipalmitoyl-glyceryl-trimethylhomoserine (DPTS) within mixed membrane systems prevalent in marine algae. CSLs, known for their toxicity and their association with Diarrhetic Shellfish Poisoning, exhibit a range of structural isomers characterized by a charged sulfate group positioned along the hydrophobic chain. Using Danicalipin A as a representative CSL and considering DPTS, a less common glycerolipid found in Ochromonas Danica, we conducted coarse-grained (CG) simulations to uncover insights into their interactions. The findings reveal that at lower CSL concentrations, the orientation and shape of the CSL molecule closely align with Moss's model(1). However, at higher CSL concentrations, various morphologies emerge. Additionally, based on the simulation outcomes, we constructed a comprehensive phase diagram for the mixed membrane system, providing an in-depth understanding of its behavior and intrinsic attributes.References[1] Moss, F. R., et al. Halogenation-Dependent Effects of the Chlorosulfolipids of Ochromonas Danica on Lipid Bilayers. ACS Chem. Biol. 2020, 15 (11)

Poster Presentation : **PHYS.P-288**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Pulsed laser-induced synthesis of cobalt selenide as bifunctional electro catalyst for total water splitting

Jayapal Anbarasan, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Multiscale structural engineering of high-performance bifunctional electro catalysts to influence hydrogen and oxygen evolution reactions (HER and OER) has a significant role in overall water splitting. Thus, we successfully designed a new strategy and synthesized cobalt selenide (CoSe) materials by pulsed laser ablation in methanol as solvent. Thus, the synthesized CoSe materials was systematically characterized by various analytical techniques viz., X-ray diffractometer (XRD), Raman, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). The electro catalytic performance of the CoSe samples toward HER and OER were tested in traditional half-cell assembly in a membrane-less three electrode configuration in 1.0-M KOH. Further, the two-electrode water electrolyzer using an optimized CoSe electrode was assembled (CoSe ‖ CoSe) for overall water splitting (OER ‖ HER) in alkaline medium. The obtained results suggest that the PLAL-assisted synthesized CoSe is a promising material for electrochemical H2 fuel production.

Poster Presentation : **PHYS.P-289**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Chemical fluctuation produced by stochastic switch with competitive versus non-competitive inactivation: A pivotal role of active state duration variability

Heemo Yang, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

Advances in single-molecule experimental technology allow to observe heterogeneity in various enzyme activity beyond the ensemble measurement. The previous theoretical approaches have succeeded in explaining turnover time distribution and its randomness parameter that classical reaction kinetics formulation cannot describe. However, there is a lack of theoretical framework to clearly explain the experimentally observed correlation between turnover times, which is beyond the scope of the renewal assumption for turnover times. In this work, we present a general matrix formulation enabling a quantitative explanation of the turnover time correlation of on-off process, which is one of the central quantities characterizing non-renewal transcription processes. Using our theory, we derive a general relationship of the turnover time correlation and burst size with the transition matrix governing transcription process, providing a physical insight into the profile of the turnover time correlation function and burst size distribution.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **PHYS.P-290**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

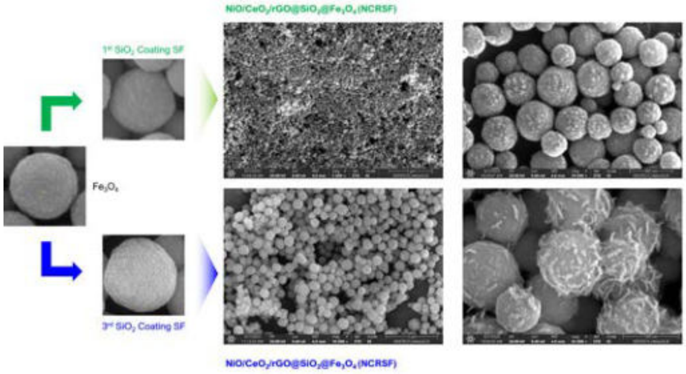
Reusable Composite Microspheres for Continuous Flow and Mass Production with Superior Photocatalytic Properties

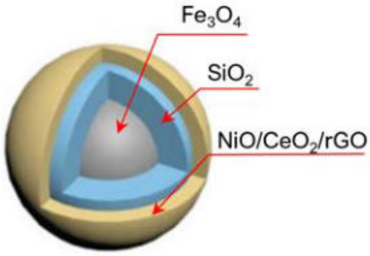
Don Keun Lee, Amol Uttam Pawar[1], Young soo Kang[1,*]

Environmental & Climate Technology, Korea Institute of Energy Technology, Korea

[1]*Environmental and Climate Technology, Korea Institute of Energy Technology, Korea*

Magnetic separation can be considered a green technology because it is fast, efficient, and consumes low energy. Hierarchical porous NiO/CeO_2/rGO@SiO_2@Fe_3O_4 (NCRSF) composite microspheres with a sandwich-like structure for a reusable photocatalyst were fabricated using an effective three-step approach. Specifically, the preformed monodisperse Fe_3O_4 microspheres were used as templates for directing the sequential deposition of SiO_2 layer by the modified Stöber method and subsequent NiO/CeO_2/rGO layer for CO_2 conversion to liquid fuels by a solvothermal method [1-3]. Intrinsic oxygen vacancies at CeO_2 surface are known to activate thermodynamically stable CO_2 molecules, enhancing the reaction rate and reducing reduction energy. However, charge recombination at the ceria-based cathode surface suppresses the multi-electron transfer process required to completely reduce CO_2 molecules to generate useful hydrocarbons. To suppress this charge recombination and facilitate the multi-electron transfer process, p-type NiO and reduced graphene oxide (rGO) were hybridized with CeO_2 to form rGO grafted NiO-CeO2 photocatalyst [4]. The phase, morphology, and structure of composite microspheres were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and FT-IR.


NiO/CeO$_2$/rGO@SiO$_2$@Fe$_3$O$_4$(NCRSF)
1st SiO$_2$ Coating SF
Fe$_3$O$_4$
3rd SiO$_2$ Coating SF
NiO/CeO$_2$/rGO@SiO$_2$@Fe$_3$O$_4$(NCRSF)


Fe$_3$O$_4$
SiO$_2$
NiO/CeO$_2$/rGO

Poster Presentation : **PHYS.P-291**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Deep Learning Strategy for Prediction of Physical Properties in Binary Chemical Mixtures

Seongmin Yoo, Jaeyoung Sung[1,*]

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

The precise prediction of physical properties in chemical mixtures is a complex task 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. Against this backdrop, this study aims to develop a deep learning-based approach to predict the physical properties of binary chemical mixtures We focus on incorporating the fraction of each component in the mixture as a key feature for prediction, aiming to provide a more accurate and computationally efficient solution. We constructed a deep learning model that utilizes graph neural networks, training the model on an extensive data comprised of both experimental and computational molecular properties. The deep learning strategy developed in this study offers a promising avenue for the accurate, efficient prediction of physical properties in binary chemical mixtures.

Poster Presentation : **PHYS.P-292**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Exploring bifunctional characteristics of Ir doped CoGa-LDH towards overall water splitting

Akash Prabhu Sundar Rajan, Senthil Raja Arumugam, 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-293**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

From PBA to Alloy: Selective Electrocatalysts for Ammonia Synthesis from Nitrite Wastewater

Ju Eun Park, Talshyn Begildayeva[1], Theerthagiri Jayaraman[1], Myong Yong Choi[1,*]

Chemistry, Gyeongsang National University, Korea

[1]Department of Chemistry, Gyeongsang National University, Korea

Electrochemical synthesis of ammonia (NH_3) attracts attention as an alternative of the Haber process owing its eco-friendliness and cost-effectiveness. Materials such as Prussian blue analogues (PBA), oxides, and alloys containing Fe, Co, and Cu transition metals were proved to enhance the efficiency of the nitrite reduction reaction (NO_2^-RR) and selectively produce NH_3 at higher yields. In this work, the series of conversions from CoCuFe–PBA, to CoCuFe oxide, and to CoCuFe alloy were achieved via successive co-precipitation, calcination, and pulsed laser irradiation in liquids (PLIL) methods. The structure of electrocatalysts was characterized by XRD and Raman, the surface chemical state was studied by XPS, the morphology was analysed via SEM, and the metals ratio was assessed by ICP-OES and SEM-EDS. The electrocatalysts showed remarkable performance in both NO_2^- degradation and NH_3 production with high Faradaic efficiency (FE) and at higher rates. The NO_2^- conversion to NH_3 product was colorimetrically detected via Griess method and indophenol blue method, respectively, and the reaction was monitored by UV-visible spectrometer. This work showed the brand-new sequential conversion of PBA to alloy via PLIL method and displayed the high performance of these electrocatalysts in beneficial application such as NO_2^-RR.

Poster Presentation : **PHYS.P-294**
Physical Chemistry
Exhibition Hall C THU 11:00~13:00

Threading Subunits for Polymers to Predict the Equilibrium Ensemble of Solid Polymer Electrolytes

Jihye Park, Won June Kim[1], YongJoo Kim[2,*], Eok Kyun Lee[3,*], Hyungjun Kim[4,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Biology and Chemistry, Changwon National University, Korea*
[2]*School of Advanced Materials Engineering, Kookmin University, Korea*
[3]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*
[4]*Korea Advanced Institute of Science and Technology, Korea*

We introduce a computational method for polymer growth called “Threading Subunits for Polymers (TSP),” which can efficiently sample solid polymer electrolyte structures cast from near good solvent conditions. The TSP method involves equilibrating subunit conformations that form favorable solvation ion shells, followed by consecutively connecting the subunits and minimizing the structures. The TSP method can sample polymers with more extended conformations and near-equilibrium structures, where ions are well-dispersed, to prevent unusual ion clustering. This leads the TSP method to substantially reduce the time required to reach equilibrium by efficiently sampling the polymer conformations near equilibrium. We expect the TSP method to be widely applied in simulations involving various types of polymer electrolytes.

Poster Presentation : **PHYS.P-295**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Preparation of antimony-doped tin oxide coating TiO2 microrods and resistance properties

Young seok Son, Don Keun Lee[1], Young soo Kang*

Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

[1]*Environmental & Climate Technology, Korea Institute of Energy Technology, Korea*

TiO2 microrods were synthesized through 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 15-30. 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. [1-2]Additionally, one-dimensional conductive TiO2 microrods coated with antimony-doped tin oxide (ATO@TiO2) were prepared using a hydrothermal coprecipitation method. Specially, sodium hexametaphosphate (SHMP) was used as an interfacial reactor to form sufficient active groups on the surface of TiO2 microrods.[3] 0.2 g ATO@TiO2 microrods 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 microrods exhibited a resistivity of (2.5 ± 0.5 KΩcm).

Poster Presentation : **PHYS.P-296**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

ZIF-8 derived N-doped porous carbon with Pt catalyst support for electrocatalytic hydrogen evolution reaction (HER) in seawater

Maheskumar Velusamy, Ahreum Min, Cheol Joo Moon, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Seawater electrolysis presents an attractive alternative to conventional freshwater electrolysis for hydrogen production, capitalizing on the abundance of seawater on our planet. However, efficient electrocatalysts for hydrogen evolution reaction (HER) in alkaline seawater remains crucial. In this study, we propose a rapid and novel method for synthesizing a highly effective electrocatalyst: metal-organic framework (ZIF-8) derived N-doped porous carbon decorated with Pt nanoparticles (NC-Pt). The NC-Pt catalyst benefits from enhanced mass and charge transport through its ordered polyhedron carbon structure and exhibits strong metal-support interaction between Pt nanoparticles and the N-doped carbon framework. As a result, the NC-Pt catalyst demonstrates remarkable activity for both alkaline and seawater electrolytes, comparable to the commercial Pt/C catalyst. The optimized NC-Pt-4 catalyst showed excellent catalytic HER performance with low overpotential of 52 and 57 mV for alkaline and seawater electrolytes at 10 mA cm-2 with amazing catalytic stability for 12 h. Notably, seawater splitting requires a slightly higher cell voltage (1.65 V) compared to overall water splitting (1.60 V) at 10 mA cm-2. The NC-Pt catalyst displays exceptional long-term stability without noticeable deterioration. This work offers a rapid and effective approach to synthesize low-cost and highly efficient electrocatalysts for alkaline seawater hydrogen production.

Poster Presentation : **PHYS.P-297**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Dual hydrogen production from electrocatalytic water reduction coupled with formaldehyde oxidation using a novel pulsed laser produced Ru/Cu composite electrocatalyst

Sagyntay Sarsenov, Senthil Raja Arumugam, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

The assembling of hybrid water electrolysis via replacing the sluggish oxygen evolution reaction (OER) with the thermodynamically more favorable formaldehyde oxidation reaction, has garnered significant attention as an energy-saving strategy for efficient hydrogen production. However, the development of highly active bifunctional electrocatalysts remains challenging. Herein, we report a novel strategy for synthesizing a Ru/Cu composite electrocatalyst using the pulsed laser irradiation in liquid (PLIL) technique. The synthesized Ru/Cu composite was systematically characterized using various analytical techniques, including X-ray diffractometry (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The electrocatalytic performance of the Ru/Cu composite toward the hydrogen evolution reaction (HER), OER, and formaldehyde oxidation reaction (FOR) was assessed in alkaline media using a three-electrode system. The obtained results suggest that the Ru/Cu composite developed through PLIL is a promising material for enhancing hydrogen production.

Poster Presentation : **PHYS.P-298**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

A novel strategy for synthesis of carbon-coated Ru nanoparticles as robust electrocatalyst for hydrazine assisted energy-saving hydrogen production

Heeeun Ahn, Senthil Raja Arumugam[1], Myong Yong Choi[1,*]

Chemistry, Gyeongsang National University, Korea

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

The hydrazine oxidation reaction (HzOR) has considered as a substitute for the oxygen evolution reaction (OER), holds promise as an efficient strategy for hydrogen production. Surface modification of Ru-based nanoparticles is widely studied to enhance surface area and achieve a synergistic effect for high electrocatalytic activity. In this work, we developed carbon-coated Ru nanoparticles using the pulsed laser ablation in liquid (PLAL) approach. Various characterization techniques, such as X-ray diffractometry (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS), were employed to analyze the synthesized samples. Electrochemical results demonstrate that the Ru/C composite exhibited a low potential of 61 mV at 10 mA cm^{-2} for the hydrogen evolution reaction in a 1 M KOH solution. Additionally, it displayed a low working potential of -0.032 V at 10 mA cm^{-2} for the hydrazine oxidation reaction in a 1 M KOH/0.5 M hydrazine solution. This study presents a novel approach to synthesizing a highly effective Ru/C composite material for energy-saving hydrogen production.

Poster Presentation : **PHYS.P-299**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Fabrication of high-entropy alloys nanostructure by pulsed laser technique for electrocatalytic hydrazine oxidation reaction

Sieon Jung, Senthil Raja Arumugam, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Electrochemical water splitting stands out as one of the most ideal methods for producing hydrogen energy to replace fossil fuels. However, large-scale hydrogen production is severely hindered by the sluggish kinetics of the anodic oxygen evolution reaction (OER). An innovative approach to achieve energy-saving co-generation of hydrogen involves coupling the electrochemical hydrazine oxidation reaction (HzOR) with the hydrogen evolution reaction (HER). Presently, the design of high entropy alloy (HEA) systems with multiple principal elements has garnered significant interest across various applications. In this study, we report the synthesis of a CoFeNiRuIr HEA with a single-phase face-centered cubic (FCC) structure using a simple and rapid pulsed laser technique. Moreover, the resulting CoFeNiRuIr HEA exhibited excellent electrocatalytic activity for both HER and HzOR in an alkaline solution. This work introduces a novel synthetic method for creating HEA electrocatalysts for large-scale hydrogen production.

Poster Presentation : **PHYS.P-300**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Nickel-Molybdenum alloy particles with pulse laser irradiation in methanol for hydrogen fuel production via water splitting

Seong Bo Lee, Hyeyeon Lee[1], Chae Eun Park[1], Theerthagiri Jayaraman[1], Myong Yong Choi[1,*]

Chemistry, Gyeongsang National University, Korea

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

The development of noble-metal-free hydrogen evolution reaction (HER) materials for electrochemical water splitting is the key to achieving low-cost and efficient electrocatalysis that drives electrochemical hydrogen evolution. Ni–Mo alloys have been previously developed for the hydrogen evolution reaction (HER), but synthesis methods to date have been limited to formation of catalyst. Here, we have fabricated NiMo alloys with various compositional ratio from the NiMo-oxide as precursor via pulsed laser irradiation in methanol process. Methanol used as solvent and also generating reducing species during pulsed laser irradiation. The synthesized materials were characterized by XRD, Raman, FE-SEM, and XPS analytical techniques, and used for hydrogen evolution reaction in an aqueous alkaline medium. Analyses indicate that the lattice distortions induced by Mo incorporation, increased interfacial activity by alloy formation, and plenty of NiMo active sites at alloy surface collectively contribute to remarkably enhanced catalytic activity. This study provides a powerful toolbox for highly efficient nonprecious metal-based electrodes for practical HER application.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **PHYS.P-301**

Physical Chemistry

Exhibition Hall C THU 11:00~13:00

Pulsed laser-assisted synthesis of Pd/NiCo$_2$O$_4$ composite electrocatalyst for energy-saving hydrogen production

Senthil Raja Arumugam, Sieon Jung, Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

Herein we report a facile strategy for the design and synthesis of Pd nanoparticles decorated bimetallic NiCo$_2$O$_4$ nanoplates as a bifunctional electrocatalyst for both HER and HzOR. Initially, the NiCo$_2$O$_4$ nanoplates were synthesized by a combination of hydrothermal reaction and high-temperature calcination. Afterward, Pd nanoparticles with varying proportions are decorated on the NiCo$_2$O$_4$ nanoplates via facile pulsed laser irradiation (PLI), leading to the formation of Pd/NiCo$_2$O$_4$ composite. The optimized Pd/NiCo$_2$O$_4$ composite exhibited a low overpotential of 294 mV(vs. RHE) for the 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. This confirms its bifunctionality in overall hydrazine splitting (OHzS) electrolyzer. As a result, the assembled OHzS with the Pd/NiCo$_2$O$_4$ ‖ Pd/NiCo$_2$O$_4$ system needs low cell voltages of 0.35 and 0.94 V to supply the current densities of 10 and 100 mA cm^{-2}, respectively. Especially, the in-situ/operando Raman spectroscopy verifies the surface formation of α-Co(OH)$_2$ during the HER and that of γ-NiOOH during the HzOR. Therefore, the synthesized Pd/NiCo$_2$O$_4$ composite could be a promising material for energy-saving hydrogen production.

Poster Presentation : **ANAL.P-302**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Considering factors for quantification of tire wear particles in environmental samples

Eunji Chae, Sung-Seen Choi*

Department of Chemistry, Sejong University, Korea

Tire wear particles (TWPs) are one of the environmental pollutants considered microplastics (MPs). TWPs are generated by the friction between the tire and road. TWPs are composed of rubber, which is a polymer, as a main component. Tire treads contain additives such as fillers, sulfur, antioxidants, and vulcanization accelerators to improve the physical and chemical properties. Pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) is mainly used for quantification of TWP in environmental samples. Pyrolysis products of rubber are used as markers for TWP. However, the same pyrolysis products (dipentene and styrene) are formed from other particles generated in the external environment, such as plant-related particles and asphalt pavement wear particles. Another critical consideration is the presence of 4-vinylcyclohexene (4-VCH), which occurs equally in BR and SBR. X-ray fluorescence spectroscopy (XRF) can be used for elemental analysis of TWP. S and Zn can be used as major markers of TWP. However, S can also be detected by external factors such as asphalt pavement and soot. Notably, when analyzing TWP using XRF, discrepancies in element concentration were observed through rubber additives and vulcanizates with known formulation. This study emphasizes the importance of considering external environmental factors when quantification of TWP in particulate matter (PM) using Py-GC/MS and XRF.

Poster Presentation : **ANAL.P-303**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Detection of drug compounds using ion mobility spectrometry: Interference by phthalates

He-Ryun Choi, Sung-Seen Choi[1,*]

Sejong University, Korea

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

Ion mobility spectrometry (IMS) is an analytical method to detect drugs in the field. Phthalates have been widely used for manufacturing polymeric items as plasticizers. Phthalates act as interferences when detecting drugs using IMS. Several drug compounds and phthalates were analyzed using IMS and their protonated molecules were observed as the characteristic ions. Product ions with different m/z values showed similar ion mobility, and their ions cannot be identified. This phenomenon can be explained by collision cross section (CCS, $Å^2$) associated with the size and shape of the ion. The CCS values at the minimum cross section of the ions were measured and their van der Waals structures were shown.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-304**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Modulation of structural chirality with magnetoplasmonic titania gel structures

Huu-Quang Nguyen, Jaebeom Lee[1,*]

Department of Chemistry, Chungnam National University, Korea

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

Hydrogel represents a category of open structure generated through the interconnected arrangement of organic or inorganic elements, leading to a loose and extremely porous configuration. The porosity of hydrogel could be fully preserved by critical point drying, which results in an ultralight aerogel structure. In this study, ultralight, magnetic translucent aerogel monoliths were fabricated from trizma-functionalized anatase (TiO_2) and magnetoplasmonic core/shell gold-magnetite composite nanowires ($Au@Fe_xO_y$ MagPlas NWs). The resulting aerogel weighs roughly 0.13 grams per cubic centimeter and showcases a wide UV-visible absorption profile, a characteristic influenced by the quantity of doped MagPlas NWs. The conjunction of the strongly UV-absorbing TiO_2 anatase with the magnetoplasmonic core-shell nanowires enhances the UV and visible light harvesting ability of the structure. Additionally, the gold-magnetite nanowires' magnetic susceptibility enables distinctive configurations within TiO_2 hydrogels by applying a helical magnetic field. Chirally active TiO_2/NWs hydrogel and aerogel have strong potential in developing applications in optics, sensing and displays.

Poster Presentation : **ANAL.P-305**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

SERS detection of natural dye molecule by metal ion-mediated bonding and NPoM

Kyunghun Kim, **Dae Hong Jeong**[*]

Department of Chemistry Education, Seoul National University, Korea

We developed a spectroscopic detection method of dyed form of natural dyestuff by combining surface-enhanced Raman scattering (SERS) and a dyeing method with metal mordant. Mimicking the surface of cellulosic fiber, gold nanofilm (AuNF) surface was modified with hydroxyl group, and then treated following dyeing process to form a chelate complex consisting of metal ion, dye, and hydroxyl group of AuNF. Then, the colloidal gold nanoparticles (AuNPs) were dropped and dried to make SERS hot-spots, where the chelate complex locates at the gap between AuNP and AuNF. For quantitative identification of enhanced signal at hot-spot, we calculated SERS enhancement factor (EF) using 4-mercaptobenzoic acid (4-MBA), and the value was 4.4×10^7. The SERS heatmap of 'dyed AuNP-on-AuNF' showed that shikonin was well bound on AuNF surface in the same way as the dyeing of dye on cellulosic fiber. Furthermore, the spectral differences were observed between 'dyed AuNP-on-AuNF' and salt-induced AuNP aggregates due to the difference in vibrational modes between dyed shikonin and free shikonin. We also suggested a possible form of dyed shikonin using density functional theory (DFT) simulation. Finally, we performed feasibility test of protocol extensibility and multiple detection, respectively. These showed that this method can be used to obtain SERS DB of natural dyes fixed on fiber, even those of mixed dyes.

Poster Presentation : **ANAL.P-306**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Study on interaction between lipid vesicle and proteins by asymmetrical flow field-flow fractionation coupled online with multi-angle light scattering (AF4-MALS)

Donggyun Kim, Seungho Lee[*], Jaeyeong Choi[*]

Department of Chemistry, Hannam University, Korea

Lipid vesicles (or liposomes) can deliver therapeutic proteins, peptides, or drugs to specific target cells or tissues. Encapsulating these substances within lipid vesicles can improve their stability, solubility, and bioavailability while controlling their release kinetics. This can lead to more effective and targeted drug delivery, reducing side effects and enhancing treatment outcomes. Therefore, understanding encapsulation efficiency is important due to the optimal formulation, quality control, bioavailability, and release kinetics. However, encapsulation efficiency is influenced by several factors, including the concentration and type of lipids and proteins used.In this study, we investigate the effect of concentration and type of protein and lipids on the encapsulation efficiency and interaction between lipid vesicles and proteins using asymmetrical flow field-flow fractionation coupled with multi-angle light scattering (AF4-MALS). As a result, free proteins (HSA and IgG) and protein-encapsulated vesicles were sufficiently separated by AF4-MALS. And the encapsulation efficiency was calculated from the separated free protein by AF4. The result was that the encapsulation efficiency increased with higher lipid concentration (1.3 → 5.2 mM) and varied depending on the protein type. In detail, IgG (11 → 20%) has higher encapsulation efficiency than HSA (3 → 13%), which is expected because IgG has more sites for interaction with lipids.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-307**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Investigating Surface Plasmon Damping and Fano Resonance Induced by Epitaxial Growth of Palladium on Single Gold Nanorods

Metya Indah Firmanti, Ji Won Ha[1,*]

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

Plasmon damping and Fano resonance induced in the growth of palladium (Pd) on gold nanorods (AuNRs) are poorly understood. Herein, we investigated the optical properties of single AuNRs@Pd (core@shell) synthesized using epitaxial Pd growth at different Pd concentrations. Core@shell AuNR@Pd demonstrated metal-induced surface damping, as evidenced by the red-shift and linewidth broadening. Addition of thiols to the bimetallic nanoparticle system revealed the competition between metal and chemical surface plasmon damping, as indicated by the real-time results of benzenethiol chemisorption involving various groups. The localized surface plasmon resonance (LSPR) spectra of single AuNRs@Pd on higher Pd concentrations showed characteristic subradiant and superradiant peaks, as well as Fano resonance as a spectral dip, which was highly influenced by the Pd shell thickness. The occurrence of Fano resonance during the Pd growth was further verified by in situ real-time observation experiments. We then elucidated time-dependent, real-time variations in LSPR peak wavelength, metal-induced surface damping, and Fano resonance mode of single AuNRs@Pd. Therefore, this study provides new insights into metal interface damping, the Fano resonance, and optical tunability by engineering Fano resonance energy and Pd shell thickness.

Poster Presentation : **ANAL.P-308**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Combined Experimental and Electronic Structure of the Optical Bandgaps of 2-D FeSe

Boka Fikadu Banti, Jaebeom Lee[1,*]

Department of Chemistry, Department of Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea, Korea

[1] Chemistry, Chungnam National University, Korea

In recent years two-dimensional materials with layered transition metal chalcogenide nanostructures reveal unprecedented electronic and optical properties due to their monolayer and electronic structure. In particular, iron selenide (FeSe) is a fascinating two-dimensional material with significant potentials, such as graphene, black phosphorus, and Mxenes in numerous technological applications to be potentially high-performance fluorophores, superconducting, and thermoelectric materials. The obtained optical band gaps from reflection electron energy loss spectroscopy (REELS) measurements were around 2.72 ~ 2.8 eV. The electrochemical analysis demonstrated the relation of band gap depending on the sample size and morphology. The obtained conduction and valence band potentials (ECB and EVB) from the reduction and oxidation onset potential of CV results of FeSe shows ECB = 5.635 eV, EVB = 4.495 eV, and Egap = 1.14 eV, respectively. Theoretical calculation approximated that the crystal structure of the bulk and a single layer of FeSe belongs to a direct band gap semiconductor with a band gap of 1.60 eV and 2.27 eV respectively. Taking the universal bridge between the normal superconducting metallic state and its Mott insulator physics state, it can be explained that the band gap instability is an effective approach to understanding the FeSe-based thermoelectric materials as well as their optoelectronic properties and may break traditional charge phase transitions and achieve feasible approach for electronic devices.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-309**

Analytical Chemistry

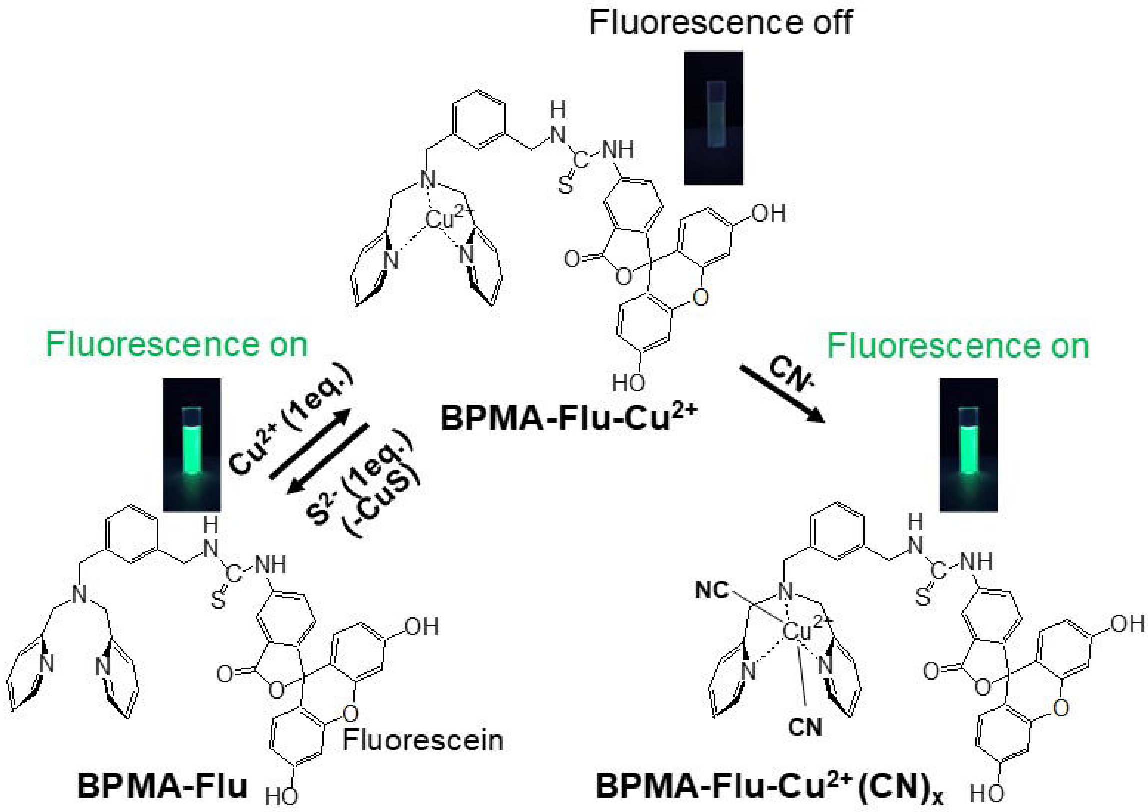
Exhibition Hall C THU 11:00~13:00

Simultaneous detection of cyanide and sulfide ions using a fluorescent chemical sensor containing a fluorophore and a potential ligand for metal complexes

Min Ji Kim, Su Bin Han, Soo Suk Lee*

Department of Pharmaceutical Engineering, Soonchunhyang University, Korea

Here, we present a fluorescent chemical sensor for the simultaneous detection of cyanide and sulfide ions, which are highly toxic to humans and environment. When the BPMA-Flu-Cu^{2+} complex comprising BPMA-Flu, a fluorophore combined with Cu^{2+}, was used, the fluorescence was turned off. However, the fluorescence was turned on again by the addition of cyanide and sulfide ions. BPMA-Flu is a unique compound containing both a fluorophore and a ligand coordinated to a metal ion. This strategy using the proposed BPMA-Flu-Cu^{2+}-based fluorescent chemical sensor facilitated quantitative analysis of cyanide and sulfide ions with high selectivity and sensitivity, despite varying detection mechanisms. The detection limit was as low as 290 nM and 74 nM for cyanide and sulfide ions, respectively. The sensor was selective and excluded other anions at concentrations 10-fold higher than cyanide and sulfide ions. The recovery rates did not exceed 10% of the original values for the detection of cyanide ions in rainwater and tap water. These results indicate acceptable accuracy and precision for practical applications.


Fluorescence off
Fluorescence on
Fluorescence on
Cu²⁺ (1eq.)
S²⁻ (1eq.) (-CuS)
CN⁻
BPMA-Flu-Cu²⁺
BPMA-Flu
Fluorescein
BPMA-Flu-Cu²⁺(CN)x
NC
CN

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-310**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

[Withdrawal] Tracing Geographic Origins Through Isotopic Ratio Analysis of Human Remains

Yu Ran Lee, Dong-Kye Lee[1,*]

Forensic Chemistry Division, National Forensic Service, Korea

[1]*Forensic Chemistry Division, National Forensic Sevice, Korea*

Poster Presentation : **ANAL.P-311**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Construction of Li-ion transport channels for practical improvement of high-voltage $LiFe_{0.4}Mn_{0.6}PO_4$ cathode material

Jimin Kim, Dung Nguyen[1], Youngil Lee[2,*]

University of Ulsan, Korea
[1]Chemical Industry Research Institution, University of Ulsan, Korea
[2]Department of Chemistry, University of Ulsan, Korea

A combination of $LiFePO_4$ (LFP) and $LiMnPO_4$ (LMP) to form $LiFe_xMn_{1-x}PO_4$ (LFMP) material has attracted much attention worldwide to further extend the driving range of the electric vehicles. However, the LFMP has low electronic conductivity and Li-ion diffusion coefficient, especially from the Mn-based domains, resulting in the satisfaction at low current rate performance. In this work, two approaches have been investigated aiming to overcome the drawbacks of the LFMP material, relying on the construction of Li-ion transport channels to practically improve the performance of the LFMP, especially at high current rates. For the first approach, $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP), a Li-ion solid electrolyte, was co-synthesized with LFMP to form LFMP-LATP composite, aiming to build the Li-ion conducting channels inside the LFMP particles. In the second approach, a hybrid coating of LATP and carbon as corresponding Li-ion and electron conducting layers on the LFMP surface to form LFMP@C_LATP was performed to simultaneously provide transfer pathways for both electrons and Li-ions. The structural and morphological characterization of the different materials was performed using X-ray diffraction and scanning electron microscope equipped with energy dispersive X-ray spectroscopy. The electrochemical properties were characterized by using galvanostatic charge-discharge and cyclic voltammetry measurements. The experimental results showed that by constructing the Li-ion transport channels, the Li-ion diffusion of the LFMP material was enhanced. In addition, the LATP provided additional capacity to the LFMP active material. As a result, the operating voltage plateaus of the LFMP material were

prolonged and stabilized. And thus, the modified LFMP exhibited excellent capacity and cycling performance.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-312**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Liquid chromatography-mass spectrometry-based approach for multiplexed and direct analysis of mature microRNAs in rat whole blood

Hyun-Deok Cho

Korea Institute of Toxicology, Korea

MicroRNA (miRNA) has recently garnered significant research attention owing to its potential as a diagnostic biomarker and therapeutic target. Liquid chromatography–mass spectrometry (LC–MS) offers accurate quantification, multiplexing capacity, and high compatibility with various matrices. These advantages establish it as a preferred technique for detecting miRNA in biological samples. In this study, we presented an LC–MS method for directly quantifying seven miRNAs (rno-miR-150, 146a, 21, 155, 223, 181a, and 125a) associated with immune and inflammatory responses in rat whole blood. To ensure miRNA stability in the samples and efficiently purify target analytes, we compared Trizol- and proteinase K-based extraction methods, and the Trizol extraction proved superior in terms of analytical sensitivity and convenience. Chromatographic separation was carried out using an oligonucleotide C18 column with a mobile phase composed of N-butyldimethylamine, 1,1,1,3,3,3-hexafluoro-2-propanol, and methanol. For MS detection, we performed a high-resolution full scan analysis using an orbitrap mass analyzer with negative electrospray ionization. The established method was validated by assessing its selectivity, linearity, limit of quantification, accuracy, precision, recovery, matrix effect, carry-over, and stability. The proposed assay was then applied to simultaneously monitor target miRNAs in lipopolysaccharide-treated rats. Although potentially less sensitive than conventional methods, such as qPCR and microarray, this direct detection-based LC–MS method can accurately and precisely quantify miRNA. Given these promising results, this method could be effectively deployed in various miRNA-related applications.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-313**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Skin-mountable and wearable colorimetric sensor for human dehydration status monitoring through sodium ion detection

Duy Nghiem Vuong, Jaebeom Lee*, Huu-Quang Nguyen[1], My-Chi Thi Nguyen

Chemistry, Chungnam National University, Korea

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

The aim of the study is to monitor electrolyte levels, particularly sodium ions (Na+) in sweat to understand the dehydration process during physical exercise or heat exposure, especially in athletes engaging in intense competition. Plasmonic-magnetic core-shell nanoparticles - Ag@Fe3O4 (Ag@Fe3O4 NPs) are synthesized using a facile one-pot one-step hydrothermal method. Afterward, 4´-Carboxybenzo-15-crown-5 is conjugated onto the surface of the as-prepared NPs to selectively bind Na+. In the presence of Na+, two adjacent crown ethers can form a sandwich-like structure with a Na+ locking pin at the center, resulting in reduced interparticle distances. The amorphous photonic arrays (APAs) are fabricated by the magnetic-induced assembly of surface-modified NPs on a polyethersulfone (PES) filter paper. The concentration of Na+ is swiftly detected by observing the color response of the APAs, induced by alteration of surface plasmon resonance properties. Later, a patch-type wearable colorimetric sensor will be developed to provide a rapid method for assessing the hydration status of athletes, enabling timely interventions to prevent dehydration-related issues.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-314**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Laser-Induced Breakdown Spectroscopy Analysis of Magneisum in Fermented Soybean Paste

Hyemin Jung[*], **Yujin Oh**[*], **Minji Kwon**[*], **Sang-Ho Nam**[*], **Yonghoon Lee**[*]

Department of Chemistry, Mokpo National University, Korea

Laser-induced breakdown spectroscopy (LIBS) is one of the simple elemental analysis techniques based on optical emission spectroscopy. It has a few unique advantages such as little-to-no sample preparation, rapidness analysis of almost all elements in the periodic table, and elemental mapping and depth profiling capability. In this work, we investigated the feasibility of LIBS as a simple technique for quantitative analysis of Mg in fermented soybean paste. Tweleve fermented soybean paste products were purchased from South Korean markets. Each as-purchased sample was freeze-dried, milled, and mixed for homogenization. A 0.5 g of the powder was taken and pressed into a pellet for LIBS analysis. Prior to the LIBS analysis, the concentration of Mg in each sample was analyzed by inductively-coupled plasma optical emission spectroscopy (ICP-OES). A laboratory-built LIBS instrument was used to record LIBS spectra. A compact low-powder diode-pumped solid-state laser and a miniature spectrometer were employed to build the cost-effective instrument. The measured Mg Ⅰ emission intensities at 285 nm showed a strong linear correlation with the Mg concentration determined by ICP-OES. A calibration curve for determining Mg concentrations between 2500 mg/kg and 9000 mg/kg was constructed based on the correlation between LIBS and ICP-OES results. Analytical performances of precison, accuracy, and limit of detection (LOD) were evaluated; precision was less than 10% in terms of relative standard deviation, accuracy was calculated to be 360 mg/kg, and LOD of Mg was estimated to be 87 mg/kg. Our results indicate that even low-performance LIBS is reliable in analyzing inorganic nutrients contained in fermented soybean pastes at the level of a few thousand parts per million and LIBS is promising as a cost-effective analysis methodology in the food industry.

Poster Presentation : **ANAL.P-315**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Localized Surface Plasmon Decay Pathways competition on Mesoporous Silica Coated Gold Nanorods Amalgamation

Yola Yolanda Alizar, Ji Won Ha[1,*]

Chemistry, University of Ulsan, Indonesia

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

This study aims to investigate the effects of mercury (Hg)-induced amalgamation and thiolation on mesoporous silica-coated gold nanorods (AuNRs@mSiO_2) by looking at LSPR single spectra and FWHM changes using Dark-Field (DF) Microscopy and Spectroscopy. First, the morphology of AuNRs@mSiO_2 exposed to Hg solution and 1-alkanethiol solution did not change due to the silica shell that prevented the AuNR core from deformation. Secondly, DF microscopy and spectroscopy observed a blue shift of the LSPR energy wavelength and plasma damping in the scattering spectra of AuNRs@mSiO_2 single particles exposed to Hg solution. Interestingly, a red shift is shown in the LSPR and a narrowing of the line width due to the strong interaction between Hg and the -SH functional group of the thiol and making a complex reaction. In comparison with expanding Hg exposed on a single AuNR@mSiO_2, the LSPR is red-shifted due to slow inward diffusion and narrowing of the FWHM. When the substrate is changed to thiol, the LSPR shows more red shift due to the strong intensity surface of the Au-Hg core shell interacting with -SH. Finally, compared to Hg exposed to the same amount of thiol carbon, the FWHM has a strong attenuation due to Au-Hg that has become an alloy that allows Au to interact with thiols. Therefore, this work presents a new strategy to study to detect Hg incorporation using the LSPR energy wavelength of AuNRs@mSiO_2 single particles and study the interfacial attenuation by looking at the interaction between Au, Hg, and -SH groups.

Poster Presentation : **ANAL.P-316**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Use of Makgeolli lees for the removal of Acid Orange 7 dye in aqueous solution

Kien Nguyen Van, Jae Jeong Ryoo[1,*]

Chemistry Education, Kyungpook National University, Korea

[1]*Department of Chemical Education, Kyungpook National University, Korea*

The objective of this investigation was to explore the effective removal of Acid Orange 7 (AO7) dye using Makgeolli lees, a common by-product obtained during the production of traditional Makgeolli beverages in Korea. A comprehensive analysis was conducted by introducing ultrasound to compare the effects of contact time, Makgeolli lees quantity, initial AO7 dye concentration, and initial pH of the dye solution with the conventional technique. The results consistently indicate that ultrasound enhances the exceptional adsorption capacity of Makgeolli lees and speeds up the process. Furthermore, the efficacy of dye removal is significantly affected by frequency, ultrasonic intensity, and acoustic power density. This study suggests that the fusion of low-cost biomass and ultrasound represents a prospective solution for the treatment of dye-contaminated wastewater.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-317**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Label-free vibrational imaging and quantification of microplastics with CARS microspectroscopy

Hayeong Lee, Hanju Rhee[*]

Seoul Center, Korea Basic Science Institute, Korea

Microplastics (MPs), broken down from plastic waste, have become a significant concern as global plastic production increases. Recently, growing attention has also been paid to the biotoxicity of nanoplastics (NPs), which are further degraded from the MPs, due to their higher potential health risk. In many studies, fluorescent-labeling methods have often been used for in vivo visualization of the MPs or NPs to study their biological behaviors. However, such a prelabeling approach has some limitations: (1) it is not applicable to the environmental MPs from nature and (2) unpredictable cytotoxicity may arise from artificially tagged fluorophores, which complicates the accurate interpretation of the inherent biotoxicity of the original MPs. Furthermore, most quantitative analyses of the MPs or NPs in biological samples rely on destructive methods that do provide only averaged information on their bioaccumulation. Label-free identification and quantification of MPs or NPs localized on specific organelles are thus essential to investigate in a systematic way their biotoxicity and impacts on organisms. In this poster, we introduce a nondestructive, label-free NP quantification method with broadband coherent anti-Stokes Raman scattering (CARS) microspectroscopy and show some experimental results obtained by combining the AFM and CARS data for self-assembled multilayers of 100-nm polystyrene beads to validate the suitability of CARS as a quantification method for NPs. More details will be discussed in the poster session.

Poster Presentation : **ANAL.P-318**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Digital and multiplexed analysis of disease-related biomarkers by integration of encoded-PEGDA microparticles and microfluidics

Minjoon Kim, Dong-Ku Kang[1,*]

Chemistry, Incheon National University, Korea

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

Polymeric hydrogel microparticles have been widely used for monitoring various disease-related biomarkers but multiplexed-monitoring is still challenge because it requires multiple probes targeting each of disease-targeting markers. To overcome such issue, graphically-encoded poly(ethylene glycol) diacrylate (PEGDA) hydrogel microparticles has attracted a lot of attention for multiplexed detection of analytes such as nucleic acid, protein, and pathogen. However, there are still challenges in sensitivity and selectivity for monitoring rare biomarkers in complexed biological samples such as blood, saliva, and urine. This bottleneck comes from high target-to-background molecules ratio since background molecules interfere target-specific reactions such as polymerase chain reaction (PCR) and enzymatic reaction. Here we introduced digital- and multiplexed-analysis of disease-related biomarkers including nucleic acid and pathogen by incorporation of encoded-PEGDA microparticle and microfluidics. Since multiplexed detection was carried with various microparticle patterns but it was not from fluorescence reporters, exponential amplification reaction (EXPAR) was conducted for multiplexed target analysis with double stranded DNA-specific fluorophore. Furthermore, microwell device was integrated where fluorescence signal is amplified under presence of target inside microwell. In the future, this platform is expected to be applied in multiplexed and digital detection for cancer mutation and viruses.

Poster Presentation : **ANAL.P-319**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Multiplexed detection of bacteria using barcoded-PEDGA microparticles

Suyeon Kim, Dong-Ku Kang*

Department of Chemistry, Incheon National University, Korea

Sepsis is usually caused by bacterial infections and is considered one of the major global causes of death. Especially, the mortality rate of sepsis is rapidly increasing due to tissue damage and organ failure without early diagnosis and treatment. Since the detection of the causative bacteria is crucial for the diagnosis and treatment of sepsis, there is a need to develop a rapid and accurate multiplexed detecting system. In this study, a sensor capable of simultaneously detecting S. aureus and E. coli, representative sepsis causative bacteria, was developed using barcode-poly(ethylene glycol) diacrylate (PEGDA) microparticles. Here, magnetic nanoparticles were also integrated into barcoded microparticles to provide magnetic property. So, the microparticles can be used for preparation of interested biomarkers. PEGDA was also carboxyl group-functionalized for probe molecule conjugation. Microparticles were then modified with capture antibodies respectively according to barcodes. The microparticles was integrated with a sandwich ELISA as a rapid and simple analysis for detecting infectious bacteria. This approach can address that the sandwich ELISA has the issue of low sensitivity by attaching HRP (Horseradish Peroxidase) conjugated antibodies on the barcode-PEGDA microparticles with captured target bacteria. The fluorescence signal was quantitatively increased by using barcode-PEGDA microparticles immobilized with HRP-conjugated antibodies, in accordance with the concentration of bacteria in the samples. This approach will be provided as an analytical method capable of rapid, accurate and multiplexed detection of disease-related biomarkers, such as bacteria, virus and nucleic acid.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-320**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Characteristics and electrochemical performance of hydroxyl-functionalized graphene quantum dot-coated Si nanoparticles/reduced graphene hybrid anodes for advanced Li-ion batteries

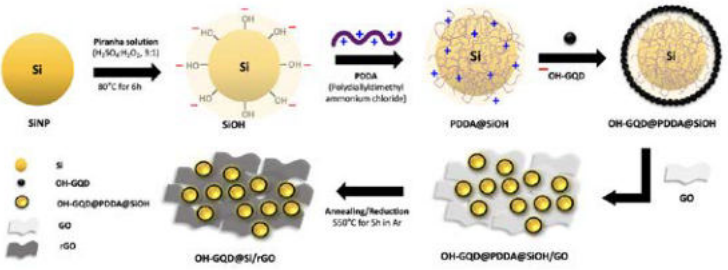
Angelica Martino, **Chang-Seop Lee**[1,*]

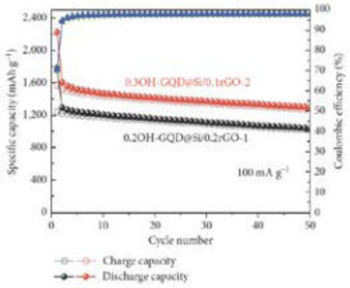
Natural Sciences / Chemistry Department, Keimyung University, Korea

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

Silicon/carbon (Si/C) composites for next-generation lithium-ion batteries (LIBs) possess tremendous potential to accelerate transition to sustainable energy sources. Herein, a double carbon protection strategy based on hydroxyl-functionalized graphene quantum dots (OH-GQD) electrostatically assembled within interconnected reduced graphene oxide networks (OH-GQD@Si/rGO) via ultrasonication and one-step, low-temperature annealing, and thermal reduction was employed to address Si low conductivity and dramatic volumetric expansion upon lithiation. The hybrid anode delivered high initial specific capacity of 2,229.16, maintained 1,090.13 mAh g−1 reversible capacity after 100 cycles and recovered 1,473.28 mAh g−1 at 5A g−1 densities. This pioneer work quantifying the synergistic benefits of OH-GQD/rGO hybridization include improved Si-rGO contact mode, stabilized electrolyte-interface formation, leading to remarkable electrochemical properties with 99.77% Coulombic efficiency. The OH-GQD carbon coating increased Li+ storage capacity through active vacancy defects and hydroxyl functionalities. Secondary protection through rGO encapsulation improved Si conductivity providing continuous electron/ion routes while buffering Si volume-induced mechanical stress. This work is expected to advance the development of future Si-based LIB anodes. The authors acknowledge funding from the Ministry of Education through National Research Foundation (Project No.: NRF-2020R1I1A3060565) and Ministry of Trade, Industry & Energy (MOTIE) through Industrial Fundamental Technology Development Program (Project No.: 20018434) of the Korean Government.

Graphical Abstract





132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-321**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Detection of SARS-CoV-2 Using CRISPR/Cas12a-based SERS Sensor

Daehyeon Kim, Hongki Kim*

Kongju National University, Korea

Developing rapid and accurate diagnostic tools for detecting severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) is crucial for effectively controlling coronavirus disease 2019 (COVID-19). In this study, we report a Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/Cas (associated protein) system-based Au nanowire (NW) surface- enhanced Raman scattering (SERS) sensor that can detect SARS-CoV-2 by adopting the Hairpin Probe-Mediated Isothermal Amplification (HIAmp) method. When the target RNA is present, the HIAmp reaction produces a significant quantity of double-stranded DNA products (FPs). Subsequently, the Cas12a/crRNA complex specifically recognizes the FPs and cleaves the Cy5-labeled single-stranded DNA linked to the Au nanowire. This cleavage results in a reduction in SERS intensity. We anticipate that this CRISPR/Cas12a-based SERS sensing method for the accurate diagnosis of SARS-CoV-2 and for broadening the application of CRISPR/Cas-based detection systems.

Poster Presentation : **ANAL.P-322**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

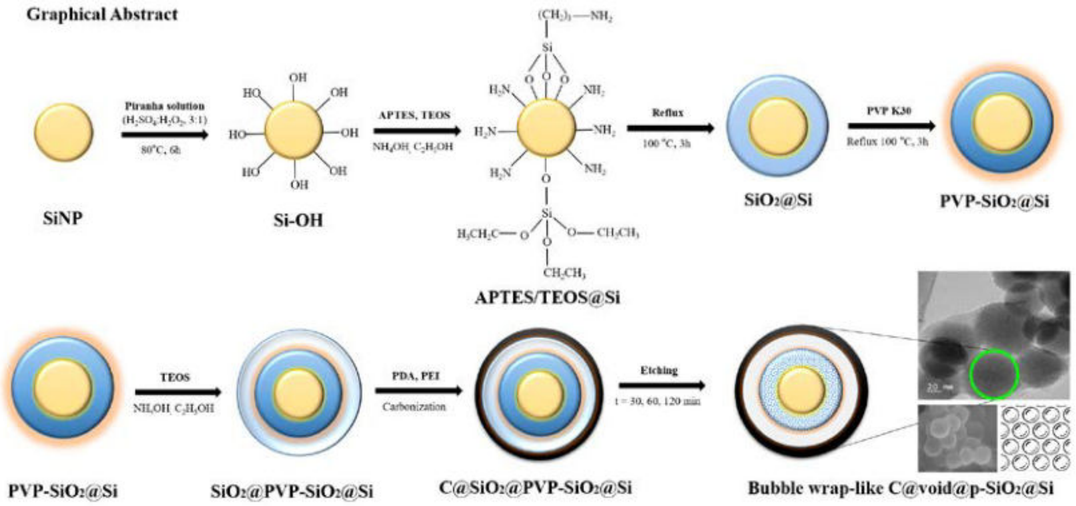
Bubble wrap-like carbon-coated rattle-type silica@silicon nanoparticles by surface-protected etching as hybrid anodes for lithium-ion batteries

Angelica Martino, Hyun Jin Kim, Chang-Seop Lee[*]

Department of Chemistry, Keimyung University, Korea

The severe volumetric expansion of silicon nanoparticles (~400%) limits its practical application as an anode material for next-generation lithium-ion batteries (LIBs). Here, we describe the fabrication and characterization of a conformal polydopamine carbon shell encapsulating rattle-type porous silica@silicon nanoparticles (C@void@p-SiO2@Si) with a tunable void structure and porosity prepared following a dual template strategy using tetraethyl orthosilicate and (3-aminopropyl)triethoxysilane (APTES) pretreated with polyvinylpyrrolidone (PVP K30) as silica sacrificial template via Stöber process. Polyethylene imine (PEI) crosslinking facilitated the construction of interconnected three-dimensional bubble wrap-like carbon matrix structure through hydrothermal-assisted carbonization by pyrolysis and subsequent selective etching. The composite anode material maintained satisfactory specific capacity after several cycles at 0.1 A g-1 and stable rate performance at high current density of 5 A g-1. The excellent electrochemical performances of C@void@p-SiO2@Si was attributed to the following: the rattle-type structure providing sufficient void space for Si volume expansion, PVP K30 pretreated silica seeds protecting Si/C spheres upon etching, carbon coating strategy increasing Si conductivity while stabilizing the solid electrolyte interface (SEI), and PEI carbon crosslinks providing continuous conductive pathways across electrode structure. The present work realizes a promising strategy to synthesize tunable yolk-shell C@void@Si composite anode materials for high power/energy-density LIBs applications.

Graphical Abstract



Poster Presentation : **ANAL.P-323**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Classification of fermented soybean pastes based on the concentrations of Mg and Sr using K-nearest neighbors

Minji Kwon[*], **Yujin Oh**[*], **Hyemin Jung**[*], **Sang-Ho Nam**[*], **Yonghoon Lee**[*]

Department of Chemistry, Mokpo National University, Korea

Fermented soybean paste is widely used as food ingredient and sauce in East Asian countries. The fermented soybean pastes, consumed in South Korea, are produced domestically or imported from China. In this work, 167 fermented soybean paste samples were collected from South Korean markets: 101 from South Korea and 66 from China. A statistical model discriminating the fermented soybean pastes produced in South Korea and China was constructed based on the Mg and Sr concentrations in the samples were analyzed by inductively-coupled plasma optical emission spectroscopy. The fermented soybean pastes from South Korea showed higher concentrations of both Mg and Sr than those from China. In the Mg-Sr variable space, two classes corresponding to the fermented soybean pastes from South Korea and China formed separated data clusters. The two-variable model performance was evaluated by k-nearest neighbors algorithm following leave-one-out validation. The classification accuracy showed a significant dependence on K, the number of voters selected from the training data set. When, k was set to 11, 13 – 16, 18, 28, 32, and 34, the classification accuracy was maximized to 90%. Also, the asymmetric numbers of training data between the two classes significantly decreased the classification accuracy when k was set to larger then 130. Our results indicate that elemental analysis and modeling based on the results can be usefully employed for origin distinction of fermented soybean paste products. This methodology would be better for practical applications than complicated isotope analysis techniques.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-324**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Determining the Electrical Surface Properties of Iron Selenide by Contact Electrification

Haheun Yoo, Jaebeom Lee[1,*]

chemistry, Chungnam National University, Korea

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

FeSe, a transition metal chalcogenide, has gained significant attention due to its unique properties, including superconductivity at ultralow temperatures. Of particular interest is the potential of two-dimensional (2D) nano FeSe to exhibit Mott-insulating behavior, displaying both insulating and conductive properties. The layered structure of FeSe nanosheets, stacked via van der waals forces, is expected to be a dielectric material showing great contact electrification. Contact electrification is the phenomenon where electric charges are generated when two different materials come into contact and then separate. This charge transfer occurs due to the difference in electron affinities and ionization energies of the materials, resulting in the accumulation of positive and negative charges on their surfaces. In this study, we investigate the surface charge of Iron Selenide by contact electrification effect through contact and separation with various counter materials. A range of materials, including FEP, PTFE, Kapton, PET, paper, aluminium, nylon were employed as counter materials in order to explore the diverse electrostatic responses induced by interactions with FeSe.

Poster Presentation : **ANAL.P-325**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Antimicrobial activity Enhancement of LPcin analogs using NMR spectroscopy

Jaewon Kwon, Minseon Kim, Yongae Kim[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Antimicrobial peptides (AMPs) are potential pharmaceutical candidates to replace antibiotics, which come with the risk of antimicrobial resistance bacteria and serious side effects. However, challenges such as establishing cost-effective mass production methods and addressing issues like susceptibility to degradation by peptidase within the in vivo condition need to be overcome. Therefore, our study aims to enhance the antimicrobial activity and structural stability of LPcin analogs, a type of antimicrobial peptide. This enhancement is achieved through metal ion binding and a cocktail strategy involving the simultaneous expression of various LPcin analogs. Metal ions play a pivotal role in stabilizing peptide structures and augmenting their interactions with bacterial membranes. Furthermore, employing a cocktail of diverse peptide analogs allows for synergistic targeting of various pathogens and reduces the likelihood of resistance development.LPcin analogs used in the experiment were LPcin-YK5, 8, 11. These analogs were obtained with high yield and high purity by optimizing expression using *E. coli* and purification using many biophysical techniques. Structural conformation was analyzed by using CD and NMR spectroscopy.

Poster Presentation : **ANAL.P-326**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Enhancement of FO-SERS sensing and quantitative detection of pancreatic cancer biomarker CA19-9 by optimization of optical fiber surface and path

Seonung Kim, Kyunghun Kim[1], Dae Hong Jeong[2,*]

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

Fiber-optic surface-enhanced Raman scattering (FO-SERS) is a powerful sensing technique that can remotely detect analyte molecules by adjusting the length of the optical fiber. However, there is a limitation in remote SERS sensing due to the strong Raman signal of the optical fiber material. To solve this problem, we improved the surface treatment and light propagation path of the optical fiber to reduce the background signal and increase the SERS signal. We also examined the effect of the connector, which is used for easy application in industrial or clinical settings, on the signal.Using these methods, we proposed a method to quantitatively detect CA19-9 (carbohydrate antigen 19-9), a biomarker of pancreatic cancer, using FO-SERS in this study. We fabricated nanoprobes by conjugating CA19-9 antibodies to 4-FBT-labeled AgNS (4-flourobenzenthiol-labeled silver nanoshell) and quantitatively applied them to the optical fiber surface using a sandwich immunoassay method with immobilized CA19-9. We observed a strong signal from the nanoprobes under the optimal Raman detection condition. We expect that this method can be used to simultaneously measure multiple biomarkers by using nanoprobes labeled with different Raman chemicals depending on the biomarker.

Poster Presentation : **ANAL.P-327**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Defining Co-resistance Mechanisms in Cytarabine-resistant Human Acute Myeloid Leukemia Cells Using Biochemical Analysis

Jinhui Kim, Sooyeon Chae

Department of Chemistry, Korea University, Korea

Acute myeloid leukemia (AML), which accounts for more than 80% of adult cases of leukemia, is a blood cancer that spreads quickly and starts in the bone marrow. For the past 40 years, combination of cytarabine (ARA-C) and daunorubicin (DNR) has been widely used as an AML treatment regimen. However, only 40% of patients who receive the ARA-C/DNR regimen achieved complete remission, and 60% of patients experience AML relapse after standard treatment. Even though there have been several studies on the mechanism of resistance to the two anticancer drugs, there hasn't been enough done on the common resistance to this two-drug regimen. We investigated the co-resistance of ARA-C and DNR in this work with the goal of elucidating this phenomenon through biochemical study. The normal AML cell line SHI-1 and the cytarabine-resistant cell line R640-SHI-1 were both treated with ARA-C and DNR separately or simultaneously, and cell viability was then measured. As a result of data analysis, It was confirmed that the R640-SHI-1 developed DNR resistance. These finding led us to assume that the R640-SHI-1 cell line not only exhibited ARA-C-specific resistance mechanisms but also a general resistance mechanism that contributed to both ARA-C and DNR resistance. To determine whether drug resistance is related to the amount of drug uptake by cells, we will measure the amount of cellular drug uptake by various analytical methods. Moreover, the co-resistance mechanism will be traced through proteomic analysis of cells, and analysis of micro-RNA components in exosomes.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-328**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Paper-based PCR platform integrated thermocycler on digital microfluidics chip

Sarath Kin, Semin Chun[1], Eunjin Huh[2], Oh-Sun Kwon[2], Kwanwoo Shin[2,*]

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

Digital microfluidics (DMF) is preferred to be used as a lab-on-a chip (LOC) device, particularly in chemistry, biochemistry, microelectronics, and molecular diagnostics. To address challenges in integrating microheaters and sensors while maintaining cost-effectiveness and eco-friendliness, we introduce a flexible paper-based DMF chip. This chip, fabricated using inkjet printing to print versatile electrodes on photopaper, integrates electrowetting-on-dielectric (EWOD), microheaters, and temperature sensors to manipulate, heat, and sense the sample droplets, respectively. Paper-based EWOD showed the ability to manipulate the sample droplets, while the printed microheater generated heat to $T > 100°C$ (meander shape of 5×10 mm in thickness of 200 μm, resistance of $R = 75\ \Omega$), and the Seebeck coefficient of thermoelectric effect of the temperature sensor was 18.87 μV/K. The combination of these components into a single paper-based digital microfluidics device can be utilized as a compact polymerase chain reaction (PCR) device for DNA amplification that is more convenient and less expensive than traditional methods.

Poster Presentation : **ANAL.P-329**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

The Artificial Circulatory System for Tumoroids (ACT): Investigating the Impact of Pharmaceutical and Biomimetic Approaches on Through MS-based Analysis

Sooyeon Chae, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Personalized cancer medicine relies on tailored treatments guided by precise scientific evidence encompassing pharmaceuticals, genes, proteins, and metabolites. Essential to this endeavor is the identification of robust biomarkers for individualized therapy.Recent research has highlighted the critical interplay between pharmacokinetics, cell biology-pharmacodynamics, and fluid mechanics within the body's circulatory system. Conventional laboratory cell-based models have fallen short in integrating these factors, leading to inconsistent drug efficacy and biomarker identification in clinical trials. Bridging this gap requires innovative pharmaceutical and biomimetic models that account for fluidic conditions.To address these challenges, we introduce the Artificial Circulatory Tumor (ACT) system, a versatile platform enabling mass spectrometry-based investigations. ACT leverages pharmacokinetic software, computer-aided design (CAD), and advanced fluid systems to construct biomimetic environments.Our study employs cutting-edge analytical techniques, including mass spectrometry (MS), computational fluid dynamics (CFD), and spectroscopy, to demonstrate the ACT's ability to replicate biomimetic pharmacodynamics. Our findings offer crucial insights into personalized cancer medicine, showcasing the ACT system's potential in biomarker discovery. By transcending the limitations of traditional laboratory models, ACT promises to expedite the development of personalized cancer treatments.

Poster Presentation : **ANAL.P-330**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

New phenothiazine-conjugated benzimidazoles for naked eye detection of Au^{3+}, Ag^{+} and Hg^{2+}

Ashwani Kumar, **Pil Seok Chae**[1,*]

Department of Bio Nano, Hanyang University, India

[1]*Department of Bionano Engineering, Hanyang University, Korea*

Phenothiazine-containing probes are rarely explored in the sensing field.[1,2] We synthesized three benzimidazole-based probes conjugated with phenothiazine (probes **1-3**) to investigate their abilities to detect metal ions in semi-aqueous media. These probes contain metal ion binding sites consisting of N and S atoms and are able to form hydrogen bonding with a protic solvent. The presence of a long alkyl chain facilitated the formation of self-assemblies of the probes in aqueous solution, resulting in effective detection of heavy metal ions (Hg^{2+}) or precious metal ions (Ag^{+} and Au^{3+}). Upon binding to the metal ion (Hg^{2+}, Ag^{+}, or Au^{3+}), the high fluorescence emission of the probe was quenched and the quenched fluorescence emission was restored upon the interaction of [probe-metal ion] complexes with a specific anion. Thus, this system enables metal ion sensing and subsequent anion sensing in aqueous media. The current study includes an investigation of the analyte binding mechanism, sensing behavior, limit of detection, and change in morphology/self-assemblies of the probes. The sensing behaviors of the probes were studied by various spectroscopic methods including NMR, UV-visible, and fluorescence spectroscopy as well as DLS, FE-SEM techniques, and DFT calculations.

Poster Presentation : **ANAL.P-331**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Gas chromatography and Paper spray ionization mass spectrometry for the analysis and differentiation of eucalyptus oils

Heejin Ro

Chemistry, Dongguk University, Korea

Eucalyptus oils have been widely used in various household chemical products including mouthwash, insect repellents, and ointments. There are more than 300 species of eucalyptus, and the commonly used types are Eucalyptus(E.) globulus, E. citriodora, and Australian types. Each of these species is listed by the International Organization for Standardization (ISO) with data on its composition and content. Chemical analysis of eucalyptus oil is typically performed by gas chromatography (GC) with mass spectrometry (MS) for qualitative analysis and flame ionization detection (FID) for quantitative analysis. In this study, we developed a method to analyze eucalyptus oil by paper spray ionization MS (PSI-MS) to find its chemical fingerprint quickly and effectively. With PSI, it can be analyzed quickly under atmospheric pressure and even with a small amount of samples. For the detection of characteristic components of eucalyptus oil, including eucalyptol and citronellal, we optimized the parameters for PSI, including spray solvent composition, spraying voltage, and paper substrate. GC-MS, GC-FID, and optimized PSI-MS were used to obtain chemical fingerprints that could distinguish the species of three different eucalyptus oils. Then, chemical fingerprint data obtained from three different analytical platforms were subjected to principal component analysis (PCA) for type-difference performance evaluation. These studies demonstrate that GC-MS, GC-FID and PSI-MS data combined with PCA could be used to determine the type of unknown eucalyptus oil and also to examine their mixing ratios.

Poster Presentation : **ANAL.P-332**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Volatile organic compounds (VOCs) capture with Deep eutectic solvents (DESs) and analysis by headspace gas chromatography mass spectrometry

Seo Young Hwang

chemistry, Dongguk University, Korea

Volatile organic compounds (VOCs), one of the substances we come into contact with the most in our daily lives, are one of the main components of air pollutants. Some VOCs have harmful effects on the human body and can cause various diseases. Therefore, it is necessary to captuere these VOCs. Absorbents that have been tested for VOCs include aqueous solutions, silicone oils, adipates, and ionic liquids. However, these absorbents are limited by poor capture efficiency, high cost, and toxicity. To address these shortcomings, green solvents called deep eutectic solvents (DESs) are emerging as a new class of absorbents for airborne VOCs. Unlike previously used solvents, DESs have the advantages of being inexpensive, easy to make, non-toxic, and have good VOC absorption efficiency. In this study, we tested the VOC absorption efficiency of various DESs and compared the performances of tested DESs to those of conventional VOC absorbents. We also developed a method for analyzing the VOCs captured in DESs using headspace-gas chromatography mass spectrometry (HS-GC-MS). DESs generally showed higher stability and capture efficiency of VOCs than conventional absorbents and thus allowed sensitive detection of trace VOCs.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-333**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Phosphoproteomic analysis to identify the mechanism underlying the development of childhood autism on prenatal VPA exposure

Hazara Begum Mohammad

Daegu Gyeongbuk Institute of Science & Technology, Korea

Autism spectrum disorder (ASD) is a heritable and heterogeneous neurodevelopment disorder characterized by impairments in social communication and interaction, sensory anomalies, repetitive behaviors, and varying levels of intellectual disability in children. ASD development has been linked to numerous genetic variations and environmental triggers. Recently, we have shown that an in vivo genetic alteration such as Cntnap2 knock-out can lead to proteome-wide change related to multiple biological processes including metabolic processes, synaptic activity, and neurogenesis, demonstrating how quantitative proteomics can help understand the underlying pathophysiology of ASD. Valproic acid (VPA) is an anti-epileptic drug to use as monotherapy and adjunctive therapy for complex partial seizures. However, it has been reported that prenatal exposure to VPA to can also lead to ASD-like phenotype. In this study, we carried out TMT-based quantitative proteomic, phosphoproteomic and CETSA analyses from neuroblastoma cells treated with VPA to discover underlying signaling mechanisms for ASD development. Further bioinformatic analysis such as GSEA and PTM-SEA using differentially expressed proteins and phosphorylations showed that various signaling pathways including Wnt signaling are altered with VPA treatment. We also found that these enriched signaling pathways play a significant role in the development of autism in children. Then, we performed TMT-based quantitative CETSA experiment to find direct targets of VPA. Several molecules including known ones have been recapitulated, and were found to be involved in signaling pathways identified by proteomics and phosphoproteomics. In conclusion, we successfully discovered the pivotal signaling pathways that lead to VPA-associated ASD development through a series of TMT-based quantitative mass spectrometry

analyses, and believe that this result can be utilized to advance an effective treatment for the abnormal behavior of ASD.

Poster Presentation : **ANAL.P-334**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Metabolic Isotope Labeling of Glycans in Fruit Fly for Quantitative Mass Spectrometry

Ye-Eun Cho, Jae-Min Lim*

Department of Chemistry, Changwon National University, Korea

One of the most popular and critical protein post-translational modifications (PTMs) is glycosylation which attaches carbohydrate to proteins. Many diseases coming from alteration of biological functions of glycoproteins which are affected by expression change in glycans. Therefore, relative quantification techniques based on mass spectrometry have been developed to analyze different glycan levels depending on the cell states. In this study, we present a straightforward and effective quantification method of N-linked glycan which is based on Metabolic Isotope Labeling with Isotopic Glucose (MIPLIG) to glycans of fruit fly (*Drosophila Melanogaster*).For efficient isotope labeling of glycans in fruit fly, a basic holidic diet was established based on the relationship between preparation of holidic nutrients and growth of fruit fly. In order to regulate all carbon sources, the carbon source of the holidic food of fruit fly was controlled by glucose with adjustable concentration, and BSA was additionally added as a pure protein source. Based on this, the optimal concentration of isotopically labeled glucose incorporated into glycan was determined, and the spectrum of isotopically labeled glycan by isotopically labeled glucose was obtained. Metabolic isotope-labeled glycomics was successfully established through area comparison of the mass spectrum of equal amounts of light and heavy glycans for relative quantitative mass spectrometry in fruit fly. To apply such analysis techniques to the fruit fly model, we established a clear experimental protocol. We cultured fruit fly larvae on a unlabeled holidic diet and isolated and purified the proteins from the larvae for subsequent glycan extraction. Mass spectrometry analysis was then conducted on the extracted glycans.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-335**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Development of phosphate ion-selective electrode for monitoring soil nutrients

SeBin Oh, Jiyeon Ha, Intae Kim[1,*], Yang-Rae Kim[1,*]

department of chemistry, Kwangwoon University, Korea

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

Phosphate is one of the essential nutrients in the soil and is used as a fertilizer in modern agriculture. However, overuse of fertilizers causes soil and groundwater contamination. Therefore, the importance of developing a real-time sensor for monitoring the phosphate concentration in the soil is emerging. An ion-selective electrode (ISE) is suitable for real-time monitoring of the concentration of phosphate ions in soil. It is more economical than colorimetric methods and does not require sample pretreatment. In addition, it is unaffected by turbidity.In this study, we synthesized a new ionophore for phosphate ions. The binding properties and selectivity were investigated by NMR titration. Then, a cyclic polyamine-based ISE was developed to monitor the concentration of phosphate ions in the soil. It is a sufficient alternative to the classical method of measuring phosphate concentration in soil.This study was carried out with the support of the Rural Development Administration of Korea Agricultural Science and Technology Development Cooperation Research Project (Project No. PJ015725032023) and the Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE) (P0020967, The Competency Development Program for Industry Specialist).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-336**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

NMR structural studies of anti-inflammatory Peptide, tIK

Jujin Park, Minseon Kim, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Previous studies have shown that the K562 (IK) protein inhibits the expression of inflammatory cytokines, and similarly, the truncated-IK (tIK) protein, a subset of the IK protein, has been shown to have the same effect. However, the high molecular weight (29 kDa) of the tIK protein has limited its drug development. To address this, we designed peptides with a lower molecular weight while retaining anti-inflammatory activity.The designed peptides are tIK-9-mer, 14-mer, and 18-mer (tIK series), which have demonstrated potent anti-inflammatory effects in preclinical studies. To understand and optimize the exact mechanism of anti-inflammatory activity of these peptides, structural analysis is required. We utilized NMR spectroscopy to investigate the detailed structures of the tIK series and their interactions with target molecules.The structural analysis of tIKs using NMR spectroscopy involved several key steps. First, we used *E. coli* to express the tIK series, and then optimized the isolation and purification process to obtain high-purity peptides. The molecular weights and purity of the purified peptides were confirmed using MALDI-TOF mass spectrometry. In addition, the secondary structures of the peptides were analyzed using spectroscopic methods such as NMR and CD. Furthermore, insights into the anti-inflammatory mechanisms of the tIK series were obtained through chemical shift perturbation. This comprehensive research approach is expected to provide important information on the structure and function of tIKs, contributing to later research.

Poster Presentation : **ANAL.P-337**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Quantification of Inorganic Mercury Using Ion-Exchange Membranes and Laser-Induced Breakdown Spectroscopy

Jang Mi Park, **Sang-Ho Nam***, **Yonghoon Lee***

Department of Chemistry, Mokpo National University, Korea

The toxicity of mercury compounds depends on the chemical structure as well as the concentration. Thus, the accurate determination of both chemical species and their concentrations in various samples has been needed to assess mercury toxicity. A new method for quantification of Hg(II) was developed using an ion exchange membrane and laser-induced breakdown spectroscopy (LIBS). Hg(II) dissolved in water was collected on the cation-exchange polymer membrane, and the membrane containing Hg(II) was directly analyzed by LIBS. The detection limit for Hg(II) was estimated to be 2.53 mg/kg. The recovery efficiency for 80 mg/kg mercury standard solutions was 104%. This method was also applied to the analysis of the certified reference material of Hg-spike water. This new method would be more cost-effective, simpler, and less labor-intensive for the quantification of inorganic mercury than the conventional chromatography-coupled elemental analysis techniques.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-338**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Improving accuracy for determination of active pharmaceutical ingredient concentration in tablets with varying compaction density using oversampling strategy

Haeseong Jeong, Hoeil Chung*

Department of Chemistry, Hanyang University, Korea

In pharmaceutical tableting process, depending on the applied compaction force, certain components may undergo physical/chemical alterations which affect their crystal structure or particle size in sequence. Therefore, these subtle changes alter the spectral features of tablets and thereby hinder the precise quantitative spectroscopic measurements. To overcome the potential degradation of accuracy under the variation of compaction density, oversampling algorithm was proposed. It was to generate multiple spectra of tablets potentially reflecting the change of compaction density in prior and use them to build a compaction density-tolerant prediction model using partial least squares (PLS). For this study, the tablets containing paracetamol as an active pharmaceutical ingredient (API) (concentration: 3 - 21%, increments of 2%) prepared with three different pressures (40, 60, and 80 kgf/cm2) were employed. Near-infrared (NIR) and Raman spectra of the tablets were collected, and these acquired spectra were combined with the spectra generated with using oversampling algorithm for the determination of API concentrations using PLS. The accuracies with and without using oversampling algorithm were mutually compared and utility of oversampling algorithm was discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-339**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Characterization of pore-forming Amyloid Beta Protein using NMR Spectroscopy

Joohan An, Yongae Kim*, Minseon Kim

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Alzheimer's disease, a progressive neurodegenerative disorder, initiates with mild cognitive decline and can ultimately culminate in the incapacitation of verbal communication and responsiveness. The pathogenesis of this debilitating condition is intimately linked to Amyloid beta (Aβ), expected to have a big correlation with Alzheimer's disease, is made from different Amyloid Precursor Protein (APP) cleavage system from normal brain. Especially, one proposed pathway of Aβ-induced neurotoxicity involves the formation of ion-channel pores within neuronal cell membranes, thereby disrupting the intricate homeostasis of intracellular calcium ions (Ca2+). Our research aims to find inhibitors that can control these ion channels by examining the structural interplay between amino acids and inhibitor functional groups. Zinc (II) ions, abundant in neural cells, present a promising option for regulating the channels. In this study, we focused on human APP containing an amino acid sequence 692-723th of the transmembrane region (hAPP-TM) which is known that it has an affinity to zinc ions. Using Solution-State NMR, we study how hAPP-TM residues interact with zinc (II) ions, revealing connections through chemical shift perturbation according to the presence or absence of zinc. Beyond this, our study elucidate the protein's structure and spatial orientation via solid-state NMR, providing insights into structural adaptations within complex lipid bilayer systems.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-340**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

A hybrid carbon/solid-electrolyte coating on Fe3BO5 conversion type anodes for ultra high C-rate applications

Rajeev Kumar, Dung Nguyen[1], Jeongin Kim[2], Youngil Lee[3,*]

Chemical Industry Research Institute, University of Ulsan, Korea
[1]*Chemical Industry Research Institution, University of Ulsan, Korea*
[2]*University of Ulsan, Korea*
[3]*Department of Chemistry, University of Ulsan, Korea*

Ultra high C-rate capability in anode materials for lithium and sodium ion batteries is highly sought after, as only few electrode materials can safely charge-and discharge for rates above 5 A/g. Among various anode candidates, Fe3BO5 (vonsenite) has emerged as a promising alternative due to its low cost and favorable electrochemical characteristics. Fe3BO5 has a high theoretical capacity (726 mAh/g), and excellent rate capability. However, challenges such as large volume expansion, irreversible capacity loss in initial cycle, voltage hysteresis, limited initial Coulombic efficiency, low electronic conductivity, sluggish reaction kinetics and poor cyclability hinder the practical implementation of Fe3BO5 in Li and Na-ion batteries. To address these limitations, researchers have explored various strategies to enhance the electrochemical performance of Fe3BO5. These include nanostructuring techniques, compositional modifications, and hybridization with carbonaceous materials or other metal oxides. Nanostructured Fe3BO5 electrodes exhibit improved lithium and sodium ion storage properties by shortening the diffusion path for these ions and accommodating the volume changes during cycling. In this work we report the use of a composite carbon/solid electrolyte (NASICON type, LATP and NATP) coating that further improves the cyclic stability of these conversion type anodes and thereby delivering at ultra high current densities of 10 A/g. The comprehensive understanding of the conversion reaction mechanism and the development of innovative strategies will pave the way for the practical implementation of Fe3BO5 in next-generation high-energy-density Li and Na-ion battery systems.

Poster Presentation : **ANAL.P-341**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

SABRE Hyperpolarization of Nicotinamide Derivatives and its Chemical Kinetic Properties

Quy Son Luu, Thi Quynh Nguyen[1], SeokKi Yun[2], Jae Hwa Choi[2], Youngbok Lee[3,*]

Bionanotechnology, Hanyang University, Korea

[1]*Department of Applied Chemistry, Department of Bionano Convergence , Korea*

[2]*Applied Chemistry, Hanyang University, Korea*

[3]*Department of Bio-Nano Engineering, Department of, Korea*

Nicotinamide derivatives play an essential role in biomedicine, such as the nicotinamide adenine dinucleotide (NAD+), which is an electron carrier in the glycolysis and citric acid cycle (known as the Krebs cycle). In addition, they are also commonly used in the production of dietary supplements (such as vitamin B3), which help us improve the appearance of fine lines, wrinkles, hyperpigmentation, and acne. Understanding the metabolism and pharmacological effects of nicotinamide derivatives is important in pharmacology. This knowledge helps in designing drug regimens and evaluating drug interactions. Hence, we utilized SABRE (signal amplification by reversible exchange) hyperpolarization using a home-built system to study the details of the pharmacokinetics of nicotinamide derivatives. This method helps us overcome the main limitation of conventional NMR (nuclear magnetic resonance), such as its low sensitivity. To prove the concept, we hyperpolarized benzyl nicotinamide (BnNCA) and nicotinic acid hydrazide (NTH). We investigated the effect of magnetic field, bubbling time, and co-ligand on the hyperpolarized efficiency of these compounds. Alongside, T1 relaxation time with and without iridium catalyst (a spin order transfer catalyst in the SABRE technique) was determined by using inversion recovery and a single shot at a small flip angle or manual method at thermal and hyperpolarization conditions, respectively. For example, the 1H NMR of BnNCA with DMSO-d6 as a co-ligand exhibited the highest enhancement factor ($\varepsilon H2 = 103$) at 6.5 mT, 90 s, and 3 atm of 50% para-hydrogen and the T1

relaxation time of proton (H2) in BnNCA and NTH at hyperpolarized is 16 s and 9 s, respectively. This long T1 relaxation time is helpful in the studying organic reaction monitoring.

Poster Presentation : **ANAL.P-342**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Improving the electrochemical performance of $Zn_3(BO_3)_2$ as an anode material for Li-ion batteries

Jeongin Kim, Rajeev Kumar[1], Youngil Lee[*]

Department of Chemistry, University of Ulsan, Korea

[1]Chemical Industry Research Institute, University of Ulsan, Korea

An anode material of a lithium-ion battery stores and releases lithium ions from the cathode when charging, which mainly affects charging speed and life. In addition, the more lithium ions that can be stored at a time can affect the improvement of the energy density of the battery, so developing a cathode material with the trifecta of density, charging speed, and durability is considered an important task. In this study, $Zn_3(BO_3)_2$was synthesized by a simple solid-state method and investigated as a conversion-type anode material. $Zn_3(BO_3)_2$is a good anode material with a theoretical capacity of 512.5 mAh/g. In addition, two types of coatings, namely electron-conducting (carbon, C) and ion-conducting (solid electrolyte, $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$, LATP), were applied to facilitate the transfer path of electrons and lithium ions for improved performance. X-ray diffraction (XRD) and electron microscopy were used for structural and morphological analysis. Electrochemical tests were performed on CR2032 type coin cells. In the rate performance $Zn_3(BO_3)_2$@C generally shows the better results. However, some interesting aspects are observed during the long cycle tests at a high rate of 1 A g-1. We observe that upto 400 cycles the carbon coated sample shows slightly higher capacity, but, beyond that the capacity fade is much more rapid compared to the LATP/C coated sample. We further tested this hybrid coated sample for fast charging applications and this material was able to sustain electrochemical activity even upto ultra high rate of 10 A g-1. Electrochemical impedance spectroscopy (EIS) results elucidate the role of an effective solid electrolyte interface in enabling a stable cycling performance even at high C-rates.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-343**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Sensitivity Enhancement of Biomolecules Detection through Flow-Controlled Lateral Flow Assays

Ignasia Handipta Mahardika, Kwanwoo Shin[1,*]

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

Lateral Flow Assays (LFAs) hold significant importance in point-of-care (POC) testing due to their ease of use, accessibility, and eco-friendliness, making them suitable for countries with limited medical infrastructure. Despite its promising potential, LFAs also present various challenges. One of the critical challenges is the isotropic wicking properties of the nitrocellulose membrane substrate, leading to inconsistent flow rates, a critical parameter affecting biomolecule reactions. In this research, hydrogel was introduced in the LFAs system. Different concentrations of poly(ethylene glycol) diacrylate (PEGDA) hydrogel were coated onto a nitrocellulose membrane, enabling the control of solution flow via customized porosity. To demonstrate the reliability of the proposed solution, the hydrogel-coated LFAs were employed for the lab-scale manufacturing of a pregnancy detection test. The hydrogel-coated LFAs exhibit sensitivity improvement through optimized hydrogel concentration, compared to the conventional LFAs without hydrogel coating. Hydrogel improves the LFAs sensitivity by functioning as flow control and additionally acts as a reservoir which leads to better control over the reaction time of biomolecules.

Keywords: lateral flow assays, hydrogel, PEGDA, flow control

Poster Presentation : **ANAL.P-344**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

CRISPR/Cas13a-mediated SERS-based dual-flow assay strips for amplification-free detection of SARS-CoV-2 RNA

Younju Joung, Soyeon Lee, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

The gold standard method for diagnosing SARS-CoV-2 target gene is RT-PCR. However, amplifying the target gene requires a 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 first channel, followed by the sequential flow of SERS nanotag solution through the second channel. This sequential flow arrangement allows for both CRISPR/Cas reaction and 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.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-345**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigation of Light-Responsive Microcapsules Based on Renewable Materials

Uyen Thi Do, Quy Son Luu, Seyoung Yang[1], Minji Song[1], Youngbok Lee[2,*]

Center for Bionano Intelligence Education and Research, Hanyang University, Korea
[1]*Hanyang University, Korea*
[2]*Department of Bio-Nano Engineering, Department of, Korea*

The escalating environmental impact of petrochemical plastics and their persistence in the environment has spurred the quest for biodegradable alternatives sourced from renewable materials. A promising contender in this regard is polylactic acid (PLA), distinguished by its biorenewable, biocompatible, and biodegradable attributes. This study investigates into innovatively incorporating azobenzene (AZO) into PLA matrices, giving rise to light-responsive PLA composites. Furthermore, a precipitation method was employed to subsequently fabricate microcapsules with on-off light-switching capabilities. Employing 1H and 13C-NMR, we probed the structural intricacies of both conventional PLA and AZO-PLA. Results reveal the successful synthesis of low-molecular-weight (L)-PLA from lactic acid monomers and confirm the integration of light-responsive AZO moieties into PLA chain, as evidenced by distinctive aromatic signals in the NMR spectra of AZO-PLA. Intriguingly, reversible photoisomerization was achieved via alternating irradiations at 365 nm and 450 nm with no apparent fatigue phenomenon, as evidenced by UV-Vis results, indicating that AZO-PLA presents good light-convertibility. Furthermore, the study characterizes microcapsules based on AZO-PLA through microscopy and NMR analyses. These findings highlight the successful generation of small spherical capsules, thus expanding the potential applications of the synthesized polymers. Looking forward, our research will elucidate the light-responsive mechanisms triggering the release of AZO-PLA-based microcapsules and explore the potential reusability of the synthesized capsules.

Poster Presentation : **ANAL.P-346**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

A Comprehensive Study of Conformational Changes in Malachite Green Using Electrochemistry-SERS

Wiyogo Prio Wicaksono, Jaeuk Ahn, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

The pH-sensitive and electroactive characteristics of malachite green (MG), a cationic dye, potentially affect the spectra of surface-enhanced Raman spectroscopy (SERS) in electrochemical SERS (EC-SERS) analysis. This study presents a comprehensive EC-SERS investigation to obtain dynamic SERS spectra of MG on Au SERS substrates at various applied potentials. Initially, cyclic voltammetry (CV) was performed on MG to determine an appropriate EC-SERS potential window, the mass and electron transfer mode involved in the redox process, and the number of electrons and protons participating. Furthermore, various parameters of EC-SERS were optimized, including pH and the type of supporting electrolytes. The results indicate that the highest SERS signal can be achieved through chronoamperometry SERS (CA-SERS) and CV-SERS at an applied potential of 0.6 V (vs. Ag/AgCl) using 0.1 M phosphate buffer at pH 4 as the supporting electrolyte. Plausible mechanisms for electrooxidation and the enhancement of the SERS signal were proposed. Interestingly, the oxidized form of MG, its conformational changes, and the transformation of adsorption orientation were successfully elucidated through CV-SERS. Finally, this work provides molecular-level insights into the adsorption orientation of MG and its oxidized form. This involves aromatic rings with a tilted upright orientation at positive applied potentials. These findings confirm a clear understanding of the enhancement mechanism of the SERS signal, which is valuable for developing EC-SERS-based MG sensing.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-347**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Developing a consumable-free peristaltic pump replacement for ICP-MS

DongChan Lee

NvisANA, Korea

Inductive Coupled Plasma - Mass Spectro scopey (ICP-MS) utilizes a peristaltic pump for sample introduction and evacuation of large droplets removed from the spray chamber. While it is possible to use a nebulizer that can self-aspirate at a constant flow rate without using a peristaltic pump for sample introduction, it is common to use a peristaltic pump to drain the spray chamber.A peristaltic pump is a device in which a tube is placed between a set of circularly arranged rollers and a pressure bar, which is pressed down, and the rollers rotate to pull or push the liquid in the tube. Due to this structure, the pump's moving parts and the liquid are separated, which has the advantage of high chemical resistance. However, because the tube is pressed and rubbed, it is deformed and worn and needs to be replaced periodically. In a typical analytical situation, this is not a difficult or time-consuming task, but in an automated system for fabrication, the simple task of replacing the tubes is a disadvantage.Therefore, Nvisana has developed a drain pump with a vacuum pump to replace the peristaltic pump for spray chamber drainage. It is as chemical resistant as a conventional peristaltic pump and does not affect the sensitivity and precision of ICP-MS analysis. It also has the advantage of not requiring regular maintenance for replacement because it does not use consumables such as tubing. It also has the advantage of being able to check the normal operation status of the pump in real time, preventing ICP-MS failure due to improper spray chamber drainage.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-348**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Preprocessing Challenges for Ultra-Trace Analysis in the Beverage

JongHo Ban, Seung Mo Nam[1], Woong-ki Kim[1], Yujin Seo[2], Siyeong Park[3], Sungyool Bong[4,*]

Water Environment, Korea Testing & Research Institute, Korea

[1]*Korea Testing & Research Institute, Korea*

[2]*Kongju National University, Korea*

[3]*Chemistry Education, Kongju National University, Korea*

[4]*Department of Chemistry Education, Kongju National University, Korea*

The Korea Food Code classifies beverages as any drinkable liquid, encompassing tea, coffee, fruit and vegetable drinks, carbonated beverages, soy milk, fermented drinks, and ginseng/red ginseng drinks. Carbonated beverages emerged as the top-selling category in 2020, constituting 30% of total sales and experiencing a growth rate of 4.2% compared to the previous year. This upward trend has remained consistent for three years. The surge in demand for delivery services, driven by the COVID-19 pandemic, has significantly boosted beverage sales, reaching approximately KRW 6,225.5 billion in 2020, representing a 1% increase from 20181. A noteworthy aspect is the potential hazards associated with the beverage manufacturing process, which involves heating and stirring and can generate by-products. Hence, strict management protocols are indispensable. For example, the addition of sugar to enhance flavor can react with residual chlorine in water used for manufacturing, resulting in the production of chlorine disinfection by-products. Consequently, it is crucial to establish an analytical method for assessing beverages. The Ministry of Environment, Republic of Korea, recommends the extraction of samples using methyl tert-butyl ether to detect the presence of chlorine disinfection by-products in drinking water2. Subsequently, gas chromatography-electron capture detection or gas chromatography-mass spectrometry is employed for analysis. It is also important to evaluate the pretreatment status of each beverage with respect to this method and devise solutions for any encountered challenges. This

study focuses on identifying issues that may arise during the preprocessing process for ultra-trace analysis and provides methods to address them.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-349**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

A Systematic Review of Volatile Organic Compounds Analysis as a Screening Tool for Breast Cancer

Ju young Kim, Yejin Park, Sunyoung Bae[*]

Department of Chemistry, Seoul Women's University, Korea

The early detection of breast cancer remains a critical challenge all over the world. Due to their distinctive metabolic signatures, volatile organic compounds (VOCs) can be promising biomarkers for various diseases such as cancer. This study employs the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) methodology to investigate the utilization of VOC analysis for breast detection systematically. By systematically searching and reviewing relevant literature from databases including Google Scholar, we identify and synthesize a comprehensive review of evidence on the diagnostic potential of VOCs in breast cancer. The review encompasses studies published within a specified timeframe, focusing on methodologies, sample types, and analytical techniques employed in VOC profiling. Initially, 2,590 studies were searched based on keywords including volatile organic compounds, disease, gas chromatography, analysis, human body odor, breast cancer, absorption, mass spectrometry, and headspace. Then, 1,130 papers were classified by including the additional keyword of breast cancer, finally leading to 49 papers. Through the PRISMA approach, this investigation provides a rigorous and transparent synthesis of existing research, highlighting current knowledge, potential research gaps, and implications for future diagnostic strategies. The outcomes of this review contribute to a better understanding of the role of VOCs in breast cancer detection and offer insight into the advancements required to translate VOC-based diagnostic approaches into clinical practice.

Poster Presentation : **ANAL.P-350**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Radical and 29Si-isotope enrichment silica nanoparticles for 29Si Dynamic Nuclear Polarization

Thi Quynh Nguyen, Seyoung Yang, Minji Song, Youngbok Lee[1,*]

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

Silica nanoparticles possess favorable characteristics for their potential use as a promising 29Si MRI probe. To fully harness the capabilities of silica material in MRI applications, the Dynamic Nuclear Polarization (DNP) technique can be effectively employed to significantly amplify NMR signals. In the present investigation, silica nanoparticles were selectively embedded with a uniform global concentration, along with a consistent 29Si-isotope ratio. These nanoparticles were strategically modified in different regions: encompassing the entire particle structure, focusing solely on the first/second 10 nm shell, or the 20 nm shell in unique onion-like configurations (core@shell@shell particles). The presence of TEMPO radicals within these particles was confirmed through EPR measurements, while the quantification of 29Si nuclei in each sample was validated using solid-state NMR techniques. These specialized particles exhibit the potential for self-polarization in DNP, and their hyperpolarization will be further investigated. This study aims to elucidate an efficient strategy for enriching both 29Si isotopes and radicals, paving the way for the advancement of 29Si MRI probe development.

Poster Presentation : **ANAL.P-351**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Comparison of the performance of thickness-tapered channel in flow field-flow fractionation with the effect of field programming in a uniform channel

Jaihoo Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Flow field-flow fractionation (flow FFF) is a elution-based method to separate particulate materials by size. In flow FFF, carrier liquid flows along the thin rectangular channel space, with crossflow acting across the channel as a driving force of separtion. Field programming in flow FFF is achieved by varying crossflow rate with time and it is efficient to elute long retaining materials in a fast time without losing resolution. However, it typically requires a special flow rate controller.Thickness-tapered channel in flow FFF was recently introduced by decreasing the channel thickness along the channel in order to increase the separation speed without using field programming and to improve separation efficiency and recovery without an expensive flow controller. In this study, the particle separation with field programming in flow FFF of uniform thickness channel is compared with the thickness-tapered channel without field programming in terms of separation efficiency and speed.

Poster Presentation : **ANAL.P-352**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Lipid perturbation in brain and spleen tissues of mice caused by SARS-CoV-2 using nanoflow UHPLC-ESI-MS/MS

Hwangyu Park, Myeong Hee Moon[1,*]

Department of chemistry, Yonsei University, Korea

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

In the 21st century, in addition to SARS-CoV-2, various other corona virus diseases such as SARS and MERS were prevalent. Due to the characteristics of continuous mutation and zoonotic infection, it is expected to remain a concern in the future. That is why the need for research is emerging because the betacoronavirus genus shows similar patterns in symptoms, infection, and metabolic pathways. Lipids play a critical role in viral entry, replication, and assembly and involve in many pathological symptoms. Therefore, lipidomic research data accumulation can aid in early diagnosis and treatment strategies. To assess how SARS-CoV-2 affects the spleen and brain tissues based on varying virus injection doses and the days post-infection, the study conducted both qualitative and quantitative lipidomic analysis at six different time points using mice infected with two different levels of plaque-forming units (PFU), comparing them to a control group. In this study, we investigated the lipid profiles of the spleen and brain tissues of SARS-CoV-2-infected mice using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry. The non-targeted comprehensive analysis identified a total of 593 and 926 lipids in the brain and spleen tissue. Notably, targeted quantification revealed significant alterations in the majority of lipids within the infected group, regardless of the infection dosage.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-353**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

NMR structural studies of Syndecan-4 and PIP_2 in cellular signaling

Minseon Kim, **Yongae Kim**[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Syndecan is a heparan sulfate proteoglycan, which is a complex between proteins and sugars present on the surface of cell membranes and is a molecule that plays an important role in the process of signaling and interaction between cells and their surroundings. Among the syndecan family, syndecan-4 functions as a structural protein while participating in several signal transduction pathways. When PIP_2 binds to the V region of syndecan-4, PKCα is activated and oligomerization of syndecan-4 is induced. The syndecan-4 dimer thus formed forms a tetramer with two PIP_2 molecules and binds to the catalytic subunit of PKCα. To study how PIP_2 binds to any amino acid in the V region and affects the structure of syndecan-4, we tried to explore it through NMR techniques. In addition, since the GXXXG motif, an amino acid sequence known to play a major role in oligomerization, is present in syndecan-4, it was confirmed whether the amino acid sequence of this motif was substituted to affect the formation of the oligomerization structure of syndecan-4. In order to obtain syndecan-4 in large quantities and conduct NMR structural studies, genetic recombination techniques were used, and structural studies were conducted using CD, MALDI-TOF, and solution/solid-state NMR with 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.

Poster Presentation : **ANAL.P-354**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

NMR structural studies of Obesity related hMC4R-TM2

Yeseul Yang, Yongae Kim[1,*], Minseon Kim[1]

chemistry, Hankuk University of Foreign Studies, Korea

[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Human transmembrane proteins (hTMPs) constituting human biological membranes, play very important roles in biological systems such as signal transduction receptor function, cytoskeleton, and cell signaling. Among them, the human melanocortin-4 receptor (hMC4R) is expressed in the hypothalamus. This is involved in appetite regulation and energy homeostasis. The heterozygous mutation of hMC4R, a substitute of the 90th amino acid, aspartic acid to asparagine (D90N) located in the second transmembrane domain (TM2), is detected in early-onset obese patients. 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). In the purification process, Sodium dodecyl sulfate (SDS) was used as a detergent because the target proteins were hydrophobic. Since SDS interferes with structural identification due to its strong binding to proteins, we removed SDS after FPLC to gain high-purity proteins. We performed various spectroscopy techniques such as CD spectroscopy, solution-state NMR spectroscopy, and solid-state NMR spectroscopy to confirm the structure.

Poster Presentation : **ANAL.P-355**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Biomarker discovery in prostate cancer from 20 cancer patients with tissue proteomics

Junghoon Kang, Miseon Jeong, Yunseon Woo, Seung Jeong Lim, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Korea

The early diagnosis of prostate cancer (PCa) is based on digital rectal examination (DRE) and/or serum prostate-specific antigen (PSA) level. However, these tests are neither sensitive nor specific enough to detect clinically significant PCa leading to overdiagnosis, such as unnecessary biopsies. This study intended to discover PCa-specific biomarker candidates from PCa tissues with shotgun proteomics for a more accurate early diagnosis.Twenty PCa tissues were collected from PCa patients with different PSA levels in blood test. The each PCa tissue was homogenized individually, and proteins were extracted using lysis buffer without detergent from the homogenized PCa tissues. Then the supernatant fluid was trypsin digested and desalted respectively, and the proteomes in each PCa tissue were identified and quantified with multiple nLC-MS/MS analyses and protein database search software. Proteomes in each PCa tissue were comparatively analyzed according to the clinical information of PCa patients, and proteins found commonly in 20 PCa tissues were identified.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-356**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Characterization of serum exosome lipids from patients with cholangiocarcinoma by nUHPLC and mFIFFF coupled with ESI-MS/MS

Hyeju Yu, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Cholangiocarcinoma carries a very poor prognosis. There are two types of cholangiocarcinoma, intrahepatic and extrahepatic. Each type has a different treatment method, so a differential diagnosis is required. Therefore, it is desired to identify potential biomarkers capable of distinguishing and diagnosing the two cholangiocarcinomas. Exosomal lipids, which are closely related to intercellular communication and have a limited size, can be useful biomarkers for lipid-related diseases.This study aims to demonstrate the potential of top-down analysis of mFIFFF-ESI-MS/MS as a high-speed screening platform by comparing the results of bottom-up analysis. Exosome lipids were analyzed through bottom-up analysis by nanoflow ultrahigh performance liquid chromatography-tandem mass spectrometry (nUHPLC-ESI-MS/MS) and top-down analysis by miniaturized asymmetrical flow field-flow fractionation and electrospray ionization-tandem mass spectrometry (mFlFFF-ESI MS/MS).Exosomes were isolated from serum samples of patients diagnosed with intrahepatic cholangiocarcinoma (ICC, n=15), extrahepatic cholangiocarcinoma (ECC, n=15), and control (C, n=15) using ultrafiltration. As a result of lipid analysis using nUHPLC-ESI-MS/MS, 966 lipids were identified, 291 lipids were quantified, and 61 lipids showing a 1.5-fold difference were selected as potential biomarker candidates. A top-down analysis will be performed on these selected targets. The Top-down analysis has been optimized to be completed in approximately 10 minutes and confirmed exosomal lipid detection.

Poster Presentation : **ANAL.P-357**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

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

Ji Yeong Lee, Hwangyu Park[1], Myeong Hee Moon[2,*]

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

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 processes result in changes in lipid composition. In this study, the recovery process from the infection 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 and 869 lipids were identified in the lung and liver samples from mice through qualitative analysis. At 1x102 PFU (plaque forming unit), most lipid classes exhibited substantial decreases in lung tissue at 2 days post-infection (dpi), followed by subsequent recovery. Similarly, at 1x105 PFU, 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. 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.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ANAL.P-358**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Rapid Forensic Analysis of Gel Pen Ink Using Capillary Zone Electrophoresis and MALDI-TOF MS

Seung Hoon Bahng[*]**, Jaeyoung Heo**[1]**, Sangwon Cha**[2,*]

Department of Chemistr, Kyung Hee University, Korea
[1]*Department of Chemistry, Dongguk university, Korea*
[2]*Department of Chemistry, Dongguk University, Korea*

Recently, the proportion of gel ink pens has gradually increased due to their usefulness despite their high prices. Basically, the composition of gel pen ink is based on water-based pigments, but partially soluble or almost insoluble. Therefore, a rapid and reliable forensic analysis technique is required for the separation and identification of gel pen ink. We used capillary zone electrophoresis for the sample of document micro-plug specimenes. A gel pen ink usually composed of a complex gel polymer, dyes and insoluble pigments. From the ink sample on paper, the soluble anionic ink dyes were directly extracted by a solution of water, ethanol, pyridine, and triton, and the extraction solution, and separated by CZE method of good resolusion using binary aqueous buffer in 10 minutes and detected electropherogram at four UV/VIS wavelengths with a diode array detector. The buffer for anionic dyes was a mixture of water/ethanol and able to separate the gel and dyes with cyclodextrine as a complexing agent. For comparison to anionic dyes, we used some soluble red and yellow dyes. The distribution of molecular weight of gel ink binder polymer was analyzed by matrix-assisted laser desorption/ionization (MALDI) mass spectrometry. Various gel ink pen samples were discriminated with the complementary data from their CZE electropherograms and MALDI mass spectra.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-359**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Microdispensers integrated with paper-based electrowetting-on-dielectric for high-precision chemical synthesis

Semin Chun, Sarath Kin, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Electrowetting-on-dielectric (EWOD) digital microfluidics has become as a powerful platform to perform on-chip droplet-based operating manipulations, such as transporting, dispensing, splitting, and mixing. Noticeably, among many platforms paper-based EWOD digital microfluidic platform can offer a simple, compact and low-cost way to fabricate droplet manipulation devices, since not only the patterned electrodes were quickly inkjet-printed on paper with conductive silver nanoparticle ink and then a dielectric polysulfone and Teflon films were spin-coated on them easily. Since droplet dispensing is a most critical drop manipulation in our developing paper-based EWOD platform, we have developed a micro-dispenser of 10 □ L capacity in order to control the liquid volume precisely. In this study we will present that gold nanorod (AuNR) synthesis has been performed using the micro-dispenser, demonstrating the capability for high precision chemical reactions on lab-on-a chip.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-360**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Optimization of skin sampling method for lipidomic analysis via nanoflow nUHPLC-ESI-MS/MS

Seunghee Shin, Myeong Hee Moon[1,*]

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

Human skin functions as a primary physical barrier against the external environment. The primary components of the outermost epidermal layer, known as the stratum corneum, consist of lipids like ceramides and glycerolipids. To efficiently sample the skin, tape stripping is commonly used, where an adhesive tape is used to collect the stratum corneum layers. Since there are several variables that affect the amount of lipids removed by each tape strip, a standardized sampling procedure is required. This study aimed to optimize skin sampling method in terms of sampling location and the number of tape strips in case of repeated stripping. Skin samples were collected from ten consecutive tape strips at the same spot, as well as from five successive tape strips at four different locations (forehead, forearm, cheek, and neck). were taken and their lipids were analyzed 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, alongside minor changes in lipid composition. This decrease became significant after the 6th strip.To overcome the strip to strip variation in lipid composition, a pooling method of different strips was adopted. Extracts from the first 3 or 5 consecutive tape strips were pooled, respectively, and analyzed. This approach resulted in the identification of over 100 additional lipid species in the pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strip 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.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-361**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Real-time and absolute quantification of rare disease biomarkers using droplet microfluidics

Sunghyun Ki, **Dong-Ku Kang**[1,*]

Chemistry, Incheon National University, Korea

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

Droplet microfluidics have been widely used as an analytical tool that can identify chemical reactions within encapsulated droplets at the single-molecule manner in analytical chemistry, analytical biology and diagnostics. Microscopic systems have been commonly used for monitoring and imaging droplets with high-magnification objective lens in confocal microscope or fluorescence microscope. However, these systems are pricey and complex for characterization of droplets in high-throughput manner to validate if it contains disease-related biomarkers such as nucleic acids, protein and pathogens. To address this issue, we introduce DropVIST (Droplet analysis system for Vast Imaging and Statistical Tool) that wide-field imaging system integrated with droplet microfluidics for a rapid and accurate droplet analysis system. The DropVIST can detect 8 different colored-droplets at a time using dFinder software, which can quantify droplets. Smallest droplet size was identified as 30 μm in diameter that can be analyzed with DropVIST and maximum detection range was characterized as 201.84 cm2 that 3,103,377 droplets can be theoretically monitored in DropVIST system at once in a real-time. In this study, DropVIST was utilized for monitoring living bacteria and it was compared with conventional approaches such as microbroth dilution and colony forming unit assay. This platform provided a rapid and accurate analytical tool that can be used for monitoring living bacteria in a single cell level.

Poster Presentation : **ANAL.P-362**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Raman spectroscopic quantification of microplastic particles in water using polydimethylsiloxane-coated nickel foam as a particle-capturing platform

Sangjae Kim, **Hoeil Chung***

Department of Chemistry, Hanyang University, Korea

Nickel foam (NF) was utilized as a microplastic particle-capturing medium in this study. NF is hydrophobic and porous, it could attract microplastic particles such as polyethylene (PE) particles and hold them inside. Nonetheless, the average recovery was 69.5% and unsatisfactory when the NF was used to capture PE particles in water samples. To increase the hydrophobicity, a circular polydimethylsiloxane (PDMS)-coated NF (PDMS-NF, diameter: 6 mm) was prepared and tested. The resulting recovery was elevated to 97.6% owing to the increased hydrophobicity of PDMS-NF confirmed by a contact angle measurement. Next, to quantify the PE particles captured by the PDMS-NF using Raman spectroscopy, a wide area illumination (WAI) scheme providing a laser illumination diameter of 6 mm was adopted to fully cover the PDMS-NF. The intensity ratios of PE and PDMS peaks in the collected spectra linearly increased with the quantities of dispersed PE particles (0.1~4.0 mg range, R2: 0.992) in water samples.

Poster Presentation : **ANAL.P-363**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

LC-MS based metabolomic analysis of plasma from a severe COVID-19 patient treated with ECMO

Yourim Shin, Youngae Jung, Geum-Sook Hwang[1,*]

Western Seoul Center, Korea Basic Science Institute, Korea

[1]*Korea Basic Science Institute, Korea*

Coronavirus disease (COVID-19) is a respiratory infection that can cause severe respiratory symptoms in some patients. In the case of severe patients, a treatment method called Extracorporeal Membrane Oxygenation (ECMO) can be considered because the oxygen supply is insufficient due to inflammation and damage to the lungs. In this study, we observed changes in plasma metabolites between individuals who survived and those who deceased following ECMO treatment using liquid chromatography tandem mass spectrometry (LC/MSMS).We collected plasma samples from 31 COVID-19 patients who received ECMO treatment between 2021 and 2022. Among these, there were total 84 plasma samples, including 52 samples from surviving group and 32 samples from deceased group, obtained at four different longitudinal time points.Partial least squares-discriminant analysis (PLS-DA) score plot generated from 60 quantified metabolites showed a separation between surviving group and deceased group. Importantly, using initial plasma samples, we observed significant changes in six metabolites between the surviving and deceased groups. Cystathionine, asparagine, arginine, phenylalanine, pyridoxine, and urea showed a decreasing trend as plasma collection rounds were progressed in surviving group. In contrast, these metabolites except for asparagine exhibited a slight increase in the deceased group.This study demonstrates that metabolomic analysis using LC/MSMS is useful for observing the plasma metabolites of deceased and surviving patients after ECMO treatment.

Poster Presentation : **ANAL.P-364**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Plasmonic Nanogap-Nanoparticles Engineered by Non-Thiolated DNAs for Highly Sensitive Nanobiosensors

Eunseo Lee, Jeong-Wook Oh[1,*]

Chemistry, Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Plasmonic nanostructures have been utilized as versatile biosensors due to their unique optical properties. Plasmonic nanogap-embedded nanoparticles create energetic "hot spots" that enable strong Surface-Enhanced Raman Scattering (SERS) signals inside the nanoparticles, providing the capability as individual nanoprobes for highly sensitive nanobiosensors. This study focuses on synthesizing plasmonic inside nanogap-nanoparticles with non-thiolated DNA. The cost-effectiveness of non-thiolated DNA provides a clear advantage over traditional thiolated DNA methods, offering a pathway to cost-efficient SERS nanoprobes. Through systematic characterization and optimization, this results would pave the way for advanced and economically viable nanoprobe systems, significantly enhancing biosensing capabilities.

Poster Presentation : **ANAL.P-365**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Untargeted Metabolomic Analysis of Liver Tissues for Mouse Infected with Covid-19

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

Western Seoul Center, Korea Basic Science Institute, Korea

[1]*Korea Basic Science Institute, Korea*

At the end of 2019, SARS-CoV-2 emerged and caused a global pandemic characterized by severe pneumonia, multi-organ failure, and death. Several studies have reported cases of acute liver damage and liver failure in response to coronavirus infection, but the hepatic metabolic changes caused by SARS-CoV-2 have not been clearly identified. This study will provide insight into metabolic pathways involved in liver dysfunction in SARS-CoV-2 infection. We obtained liver tissue samples from hACE2 mice intranasally infected with 10^2 wuhan virus at 2 dpi, 5 dpi, 7 dpi, 14 dpi and control (no infection). Analysis of liver tissue from SARS-CoV-2 infected mice was performed by untargeted metabolomics approach using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS). The Principal Component Analysis (PCA) score plots, a supervised multivariate data analysis method, was conducted to examine differences according to dpi in both the positive and negative ion mode. And then, kruskal-wallis test was performed and a total of 75 metabolites showed significant changes after infection with SARS-CoV-2. K-Means Clustering was performed to confirm the tendency, and it was possible to confirm the pattern of increasing after 7 day, decreasing pattern after 7 day, and increasing pattern from 2 day to 14 day. Through these pattern changes, it can be confirmed that various metabolic changes occur in the liver after infection. The results of this study suggest that LC/MS-based untargeted metabolomics can be a useful tool for understanding hepatic metabolic changes caused by SARS-CoV-2 infection.

Poster Presentation : **ANAL.P-366**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

LC-MS-based lipidomics reveals disrupted lipid metabolism in macrophages exposed to particulate matter

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

Western Seoul Center, Korea Basic Science Institute, Korea

[1] *Korea Basic Science Institute, Korea*

Particulate matter (PM) is a major environmental concern worldwide and has been reported to cause health problems including diabetes and atherosclerosis. Emerging evidence suggests that macrophages, as innate immune cells, play a key role in regulating lipid metabolism within biological systems. However, studies on the underlying molecular mechanisms linking PM exposure and its impact on cellular responses such as lipid metabolism and inflammation are poorly understood. In this study, we investigated PM-induced lipidomic changes and their associations with inflammation in macrophages. Raw 264.7 macrophage cells were exposed to PM10-like fine dusts (CZ100) and PBS (control group). Then, the extracted lipidome of macrophage cells was profiled using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry. As a result of multivariate analysis, the principle component analysis score plots showed clear separations between CZ100 and PBS groups. And, we observed significant alterations in the lipidomic profiles of macrophatges exposed to PM. Specifically, the levels of lysophosphatidylcholines, lysophosphatidylethanolamines, ceramides and very-long chain fatty acids were remarkably increased in CZ100 cells compared to PBS cells, whereas those of plasmanyl-phosphatidylethanolamines and phosphatidylinositols were significantly decreased in CZ100 group. These lipidomic changes were have been widely reported to be associated with macrophage inflammation. Therefore, our findings suggested that PM exposure induced disruption in lipid metabolism and classical activation in macrophages, resulting in a pro-inflammatory phenotype.

Poster Presentation : **ANAL.P-367**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Vibrational Circular Dichroism for analysis of metal chalcogenide nanoparticle

Yujin Choi, Jaebeom Lee[1,*]

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

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

The employment of metal chalcogenide nanoparticle enclosed by ligands, exhibiting a circular dichroism (CD) peak within the near-infrared (NIR) range, offers a promising path for optical investigations. Their remarkable optical characteristics, adjustable CD reaction via ligand manipulation, and harmonious interaction with biological systems bestow them with a versatile foundation for a diverse array of applications. This propels progress in realms like biological visualization, detection, and the innovation of sophisticated optical apparatus. The ongoing exploration and refinement of the optical traits of FeSe quantum dots capped with chiral ligands carry substantial potential to expand the frontiers of optical research, facilitating revolutionary breakthroughs across multiple scientific and biomedical domains.

Poster Presentation : **ANAL.P-368**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Band gap analysis of FeSe nanomaterials with diverse dimensions using optical method

Hyojin Kang, Yujin Choi, Jaebeom Lee[1,*]

Chemical engineering and Applied chemistry, Chungnam National University, Korea

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

Metal chalcogenides, including molybdenum sulfide (MoS2), nickel sulfide (Ni3S2), and copper-based chalcogenides, are predominantly characterized by a two-dimensional structure and have been subjects of extensive study across diverse fields over the past decade. The recent discovery of two-dimensional atomic crystals showcasing intricate photonic and optoelectronic properties has rekindled interest in the advancement of next-generation optoelectronic devices. Among these, FeSe superconductors and related transition metal chalcogenides have garnered attention due to their distinct properties. Emerging as semiconductor light emitters, FeSe quantum dots have exhibited compelling traits, such as multi-colored excitation-dependent emission (MEDE), attributed to unique electronic states. Our research delves into FeSe nanocrystals with varying sizes and morphologies, revealing unconventional band gaps and optical behaviors. This exploration further uncovers size and shape-dependent characteristics, unearthing novel phenomena like room temperature phase transitions and band gap instabilities arising from correlated orbital interactions. This innovative methodology bears the potential to decipher electronic band structures, disrupt charge phase transitions, and propel the evolution of electronic device technology.

Poster Presentation : **ANAL.P-369**
Analytical Chemistry
Exhibition Hall C THU 11:00~13:00

Advanced Solution NMR Spectroscopy for Comprehensive Characterization of Crystalline Phases in Poly(vinylidene fluoride) (PVDF) for Good-performance Electrode

SeokKi Yun, Jiwon Kim[1], Quy Son Luu[1], Youngbok Lee[1,*]

DEPARTMENT OF CHEMICAL AND MOLECULAR ENGINEERING, Hanyang University, Korea
[1]*Department of Bionano Technology, Center for Bionano intelligence Education and Research, Hanyang University, Korea*

Poly (vinylidene fluoride) (PVDF) is a versatile dielectric polymer used in lithium-ion batteries and chemical equipment. It exists in four crystalline phases (α, β, γ and δ) with varying electrical responsiveness. Studies primarily focus on its efficiency as a binder through surface and electrochemical analyses but lack depth in examining cycling and polymorphic effects. In this study, we aim to develop a solution NMR-based technique for assessing the fine structure and crystallinity of PVDF materials, laying the foundation for high-performance PVDF binder material development and the establishment of a PVDF material database. As a first step, commercial PVDF samples were separated into α, β, and γ phases using various recrystallization techniques to gather information on their structure and crystallinity. The samples underwent recrystallization under varying solvent, drying temperature, heating rate, and drying gas conditions, and were analyzed via 1H and 19F NMR to determine their primary structures, including the presence of defects, and calculated H-T/H-H ratios. Subsequently, variable temperature-NMR experiments were conducted to observe temperature-dependent changes in the PVDF structure and crystallinity. After that, T1 and T1rho relaxation analyses were performed to assess the thermal stability and structural changes in the samples. Furthermore, to elucidate the detailed spatial structural information and the relationships between crystallinity phases (α, β, γ), analyses including 19F-19F selective COSY and 13C-19F HSQC were carried out. These research findings demonstrate the potential for effectively

utilizing solution NMR in evaluating the fine molecular structure and crystallinity of binder materials, which are directly linked to electrode performance.

Poster Presentation : **ANAL.P-370**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Metabolic and immunological responses to Delta and Omicron variant infection in hamster lung tissue

Sunho Lee, Jueun Lee, Geum-Sook Hwang[1,*]

Western Seoul Center, Korea Basic Science Institute, Korea

[1]*Korea Basic Science Institute, Korea*

Coronavirus (COVID-19) has been continuously as an ongoing pandemic, with an increasing variety of viral variants emerging over time and shorter intervals between their appearances. The coronavirus directly infects the lungs, significantly impacting the immune system by modulating metabolic changes and triggering a cytokine storm. Additionally, various inflammatory cytokines are known to increase as the severity of coronavirus infections rises. However, the research on the relationship between virus infection-induced metabolic changes and the immune system is currently lacking.In this study, we performed metabolic profiling in hamster models using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS) to investigate metabolic changes after infection with the Delta and Omicron variants compared to pre-infection. The changes of cytokine levels derived from RNA sequencing data were examined to gain insights into their role in the immune response to SARS-CoV-2 variants. And then, we explored the associations between metabolic changes and inflammatory cytokines.In the metabolic profiles, arginine biosynthesis was significantly altered in both Delta and Omicron variants, while glutathione metabolism and tryptophan metabolism were significantly changed only in the Delta variant. For the alterations in cytokine levels, CCL5, CCL8, CSF1, and TNFAIP8L2 exhibited significant increases in both variant groups, whereas CCL4, CCL7, CXCL10, and IL-1β showed a substantial increase in the Delta group compared to the Omicron group. In the Delta variant, arginine exhibited significant positive correlations with CCL4 and CCL5, and proline and glutathione showed positive correlations with IL-12B. Glutathione oxidized displayed positive correlations with CCL7 and CCL8. In the Omicron variant, aspartate and ornithine

were negatively correlated with CCL8 and TNFAIP8L2, respectively. In addition, proline exhibited negative association with CCL5 and CSF1 in the Omicron variant.These findings suggest that SARS-CoV-2 variant virus infections induce distinct metabolic changes and inflammatory responses, and changes in metabolic pathways can undergo modification due to the influence of the immune system within the lung of hamsters. This study can provide valuable insights into the altered metabolic pathways and immune system changes influenced by the Delta and Omicron variants.

Poster Presentation : **ANAL.P-371**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Investigation on Microbial Degradation of Biodegradable Microcapsules Using 1H-NMR

Ye Eun Park, Jiwon Kim[1], Uyen Thi Do[1], Seyoung Yang, Youngbok Lee[2,*]

Department of Applied chemistry, Hanyang University, Korea

[1]*Department of Bionano technology, Hanyang University, Korea*

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

As pollution in the marine environment by microplastics becomes more serious, research on the field of eco-friendly polymer-based materials that can replace microplastics is becoming more active. Among them, microcapsules have the advantage of being able to control the release of the key substances, which has attracted attention especially in the cosmetic field and drug delivery system. With the development of these biodegradable capsule materials, it has become important to develop the biodegradability pre-screening method on the lab-scale for obtaining information on the degradation mechanism to improve their properties. In this study, we aimed to degrade natural polymer-based microcapsules using Enterobacter xiangfangensis (PP 2), which are known to degrade biodegradable polymer, and observe them using NMR. Microcapsules synthesized with sodium alginate and gelatin as wall materials were used in this research. To induce biodegradation, microcapsules were cultured with microorganisms known to degrade plastic. At specific times, the mixture was taken by a certain volume, centrifuged, and this sample was measured by NMR. To determine actual biodegradability, experiment were conducted with/without microorganisms. While the control sample did not show any significant changes in the NMR spectrum, the microcapsules incubated with microorganisms showed changes in the spectrum over time. Furthermore, BOD and microscopic analysis were performed simultaneously to demonstrate morphological changes caused by microorganisms. These results identified that the microbial degradation of microcapsules appeared as changes in NMR spectrum, and the possibility of measuring biodegradation through NMR analysis was verified.

Poster Presentation : **ANAL.P-372**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Comprehensive profiling of PHF6 T208-induced interactome to seek mechanism hints of its epigenomic dynamic changes in breast cancer

Jiwon Hong, Somi Jeong, Sang-Won Lee*

Department of Chemistry, Korea University, Korea

Histone modification is known to produce epigenetic changes along with DNA methylation. If induced properly, this could enable an effective change of cell fate in a desired direction. A material T208, was engineered to effectively induce such histone modifications. When applied to PHF6, PHF6 T208 has shown to effectively reduce a well-known oncogene β-catenin, in MDA-MB231 breast cancer cell-line indicating different chromatic dynamic than that of wildtype. However, detailed information on the PHF6 T208-induced interacting proteins contributing to such effect remains unclear.In this study, a comprehensive profiling of the interactome between wildtype PHF6 and PHF6 T208 was compared in MDA-MB231 by employing a modified TurboID enzyme capable of desthiobiotin and biotin proximity labeling. Three replicates of each condition were in-solution digested then taken for biotinylated and desthiobiotinylated peptide enrichment with streptavidin immunoprecipitation. Label-free quantification using a home-built dual online LC system combined with Exploris480 Orbitrap mass spectrometer was performed for all six samples respectively. With application of accurate mass tag retention time database (AMTDB), LC-MS/MS data resulted in a total of 31,622 desthiobiotinylated and biotinylated peptides corresponding to 4,951 proteins. We plan to further investigate differentially expressed protein interactome candidates based on the obtained quantification results to find hints in the mechanism of the role of T208 material contributing to epigenetic changes in breast cancer.

Poster Presentation : **ANAL.P-373**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Chemical characterization of aerosol particulate matter with UHR-MS and Neural networks from Road, Subway, and Urban Sources

Geondo Park, Seungwoo Son[1], Yong-hyeon Yim[2], Sunghwan Kim[3,*]

department of chmistry, Kyungpook National University, Korea

[1] *Chemistry of department, Kyungpook National University, Korea*

[2] *Inorganic Metrology Group, Korea Research Institute of Standards and Science, Korea*

[3] *Department of Chemistry, Kyungpook National University, Korea*

Aerosol particulate matter(APM), has become a major environmental concern due to its harmful effects on human health and ecosystems. The samples for this study were collected from roads in Daejeon and Seoul cities, as well as from subways. In this study, we search into the negative effects of APM and assess its impact on the quality of life. To analyze the water-insoluble compounds present in the collected APM, we utilized a combination of Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS), ultra-performance liquid chromatography (UPLC), and atmospheric pressure chemical ionization (APCI)(-). Furthermore, we employed gas chromatography-mass spectrometry (GC-MS) to investigate the polycyclic aromatic hydrocarbons (PAHs), utilizing a mixture of 22 PAHs. The samples were collected over a two-year period from 2019 to 2020. The complex mass spectrometry data were deciphered using an artificial neural network (ANN). For validity and accuracy, 18 samples were analyzed in six replicates using UPLC APCI(-) FT-ICR MS. Principal component analysis (PCA) was performed to demonstrate high reproducibility and statistical significance across roads, subways, and city centers. Double bond equivalence (DBE) plots revealed the presence of oxidized PAHs-like structures on the roadway, while in the city center, non-aromatic compound-like structures were observed. Vankrevelen diagrams confirmed the location-specific origin of the compounds. The quantitative analysis data of PAHs were utilized to evaluate the recovery rate and determine the concentration of toxic substances in

APM. The results of this study will contribute to an improved understanding of APM pollution and the mitigation of its adverse health and environmental impacts.

Poster Presentation : **ANAL.P-374**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Band gap Estimation of 2D Multilayered FeSe nanoplates using Cyclic Voltammetry

Jae Kyung Lee, Jaebeom Lee*

Chemistry, Chungnam National University, Korea

The iron selenide (FeSe) is well-known as a superconductor at cryogenic temperature (8 ~ 40 K). However, instead of its superconductive properties, another intrinsic characters did not receive significant attention in the academic field. Recent reports stated that FeSe has considerable size of band gaps. Kwon et al(1) already described the FeSe nanoparticles, 3 ~ 4 nm size, coupled by L-cysteine appeared multi-colored excitation dependent emission for photoluminescence, and the nanoparticle's band gaps are estimated around 1.82 eV by DFT calculation and 2.44 eV by Kubelka Munk transformation from UV-Vis spectrum. In the more previous years, many experiment results were also reported to estimate the band gap of FeSe with various synthesis method and achieved size using Tauc plot from UV-Vis absorbance spectrum. In spite of such attempts to define the band gap of FeSe, the collected band gap values showed big differences between them. Herein, cyclic voltammetry (CV) was applied to estimate the band gap in organic solvent with nitrogen atmosphere, which is generally used method to define the band gap of semiconductive organic compounds or inorganic quantum dots. To make sure the resulf from CV, ultraviolet photoelectron spectroscopy (UPS) and reflectance electron energy loss spectroscopy (REELS) were also investigated to estimate the band gap of FeSe in optical method. From the experiments, we could estimated that the band gap of FeSe in electrochemical analysis (CV) was almost 1.05 eV, when the value using photoelectron spectroscopy was around 2.72 ~ 2.8 eV. (1) Nano Today 43 (2022) 101424

Poster Presentation : **ANAL.P-375**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

photoelectrocatalysis Effects of IrO_2 cocatalysts on $SrTiO_3$ nanocubes

Hyun Ju Yang, Jinju Kim, Je Hyun Bae*

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

Forming a heterojunction structure by loading a co-catalyst on the photocatalyst is one of the methods that can lead to the highest efficiency of the photocatalyst. $SrTiO_3$ with a cubic structure was prepared using a single-step hydrothermal method in this study. In addition, $IrO_2/SrTiO_3$ heterojunction structures were prepared by loading IrO_2 on the surface of $SrTiO_3$ by controlling the amount of Ir precursor through the impregnation method. The prepared material was analyzed using TEM(Transmission Electron Microscopy) to confirm the morphology, and it was observed that IrO_2 was well loaded on $SrTiO_3$ surface. In addition, the XPS (X-ray Photoelectron Spectroscopy) analysis result showed that IrO_2 clearly exists, as a peak value consistent with IrO_2 was observed at a specific binding energy. The photoelectrocatalytic activity of the synthesized nanocatalysts for photoelectrochemical water oxidation was investigated using linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS). It was confirmed that IrO_2 nanoparticles plays a good role as cocatalysts on the nanocubic $SrTiO_3$ surface for OER (Oxygen Evolution Reaction).

Poster Presentation : **ANAL.P-376**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Voltage-programmed Capillary Gel Electrophoretic Separation for the Fast Screening of PCR Products of Severe Acute Respiratory Syndrome Coronavirus 2 with High Sensitivity

Changuk An, Seong Ho Kang[1,*]

Chemistry, Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Fast and highly sensitive detection has become essential to prevent the transmission of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). However, accelerating the analysis often leads to compromised precision and accuracy. This research aims to investigate a fast and highly sensitive screening technique for identifying polymerase chain reaction (PCR) products of SARS-CoV-2 using voltage-programmed capillary gel electrophoresis. By separating and identifying the PCR products related to the RNA-dependent RNA polymerase (RdRp) and spike (S) genes, we successfully diagnosed cases of coronavirus disease 2019 (COVID-19) within just 4 min using this method with strong dependability and precision. This indicates an acceleration of at least 7.5 times compared to previous COVID-19 diagnostic methods. The limit of detections for RdRp and S gene fragments were 1.34–3.46 pM. The developed approach is variously applicable, enabling the analysis of PCR products with specific DNA sizes and the identification of SARS-CoV-2 mutations without reducing resolution. Furthermore, it can also be applied to the fast analysis of DNA molecules associated with various infectious diseases.

Poster Presentation : **ANAL.P-377**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

EGaIn Liquid Metal and Au Hetero-Plasmonic Nanoparticles

Seoyoung Hur

Department of Chemistry, Hankuk University of Foreign Studies, Korea

In recent years, gallium-based liquid metals (LMs) have attracted numerous studies due to their low viscosity, low toxicity, and high electrical conductivity. Notably eutectic gallium-indium (EGaIn) LM nanoparticles (NPs) are of interest for their potential application in UV plasmonics and biomedical imaging and therapeutics. However, surface modification is still challenging, and the optically active range is confined in the UV region (not expanded to the visible and IR range), making it troublesome for wide applications. In this study, we synthesized novel hetero-plasmonic structures with liquid metal (EGaIn) and noble metal (Au), and the optical properties were engineered by controlling the composition of EGaIn and Au.

Poster Presentation : **ANAL.P-378**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Plasmon-Driven Catalytic Performance of Au/Pd Core-Shell Nanoparticles and Mechanistic Insights

Lucas Cho

Department of Chemistry, Hankuk University of Foreign Studies, Korea

The catalytic prowess of palladium (Pd) in various chemical reactions is widely recognized; however, its plasmonic properties are less pronounced compared to coinage metals such as gold, silver, and copper. To synergize substantial catalytic activity with enhanced plasmonic characteristics, we have engineered heterometallic Au/Pd core-shell structures. By precisely tailoring the thickness of the Pd shell, we have developed a highly efficient plasmon-mediated photocatalyst. This innovative design has been substantiated through meticulous in-situ Raman spectroscopy, which provided compelling evidence of plasmon-enhanced catalytic reactions. Furthermore, our investigation delves into elucidating the mechanistic insights underlying these plasmon-enhanced photocatalysts. This endeavor involves a comprehensive analysis of catalytic behaviors contingent upon the specific wavelengths of the employed laser. Our study not only sheds light on the intricate interplay between catalysis and plasmonics but also offers a promising avenue for the development of advanced plasmonic photocatalytic systems.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ANAL.P-379**

Analytical Chemistry

Exhibition Hall C THU 11:00~13:00

Laser induced damage of nanoplastics during Raman detection

Juhui Seo

Inha University, Korea

Nanoplastics(NPs) are growing concerns due to their potential health and environmental implications, prompting the investigation of various detection methods. Among them, Detection methods for NPs, such as MS(Mass spectrometry), SEM(Scanning electron microscopy) and TEM(Transmission electron microscope), often require destructive techniques like high vacuum, surface coating, or thermal decomposition. In contrast, Raman spectroscopy, which non-destructively provides the information of molecular fingerprints, is a promising analytical method for NPs analysis. However, the optimal experimental design for NPs analysis using Raman spectroscopy is not yet be firmly established. In this study, we examined the effects of laser irradiation on nanoplastics used in Raman spectroscopy measurement. We injected well-controlled laser power into standard polystyrene spherical particles, revealing significant changes in particle shape and signal reliability. Utilizing Dark field-based Raman spectroscopy, individual particles are injected precisely controlled laser power density. We showed that NPs undergo melting, deformation, or even combustion with increasing laser power, disrupting the reliable detection of NPs. The critical laser power required for such effects is often lower than that used in many microplastics detection Raman spectroscopy studies. Our results emphasize the necessity of establishing appropriate experimental conditions, considering the physical properties and laser power effects of nanoplastics. We suggest that comprehensive consideration of factors such as laser power, wavelength, particle type, and size to fully use the advantages of non-destructive Raman spectroscopy for precise NPs analysis.

Poster Presentation : **LIFE.P-52**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Investigation on Chemical Inhibitors of Starch Excess 4

Youngjun Kim

Medicinal Bioscience, Konkuk University, Korea

Starch, a major storage carbohydrate in plants, is a food resource that is produced in large quantities worldwide, and plants that are an important source of starch include corn, wheat, potato, cassava, and sweet potato. Starch is used as such in the food field, and only starch is extracted to give various functions to food as a substitute for gelatin or gum. Recently, biofuels have been attracting attention as alternatives to fossil fuels that cause environmental pollution. Accordingly, there is an increasing demand for enhancing starch content in plants. Starch degradation in plants requires reversible glucan phosphorylation by dikinases and phosphatases on the surface of starch granules in plant chloroplasts. Among phosphatases, Starch Excess 4 (SEX4) dephosphorylates the C3 and C6 positions of glycosyl residues in starch to allow starch degradation, so starch dephosphorylation by SEX4 is essential for starch degradation. SEX4-defective plants contain more starch due to inhibition of starch degradation, resulting in starch accumulation. Until now, genetic modification has been known as a technique to reduce the activity of SEX4, but there has been a problem with safety because the side effects of genetic modification have not been reviewed. Therefore, there is a need for a technique for increasing starch content in plants by reducing SEX4 activity without genetic modification. We are trying to get the chemical inhibitors of SEX4 and presenting the screening results of SEX4 with chemical library to increase starch content in plants.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-53**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

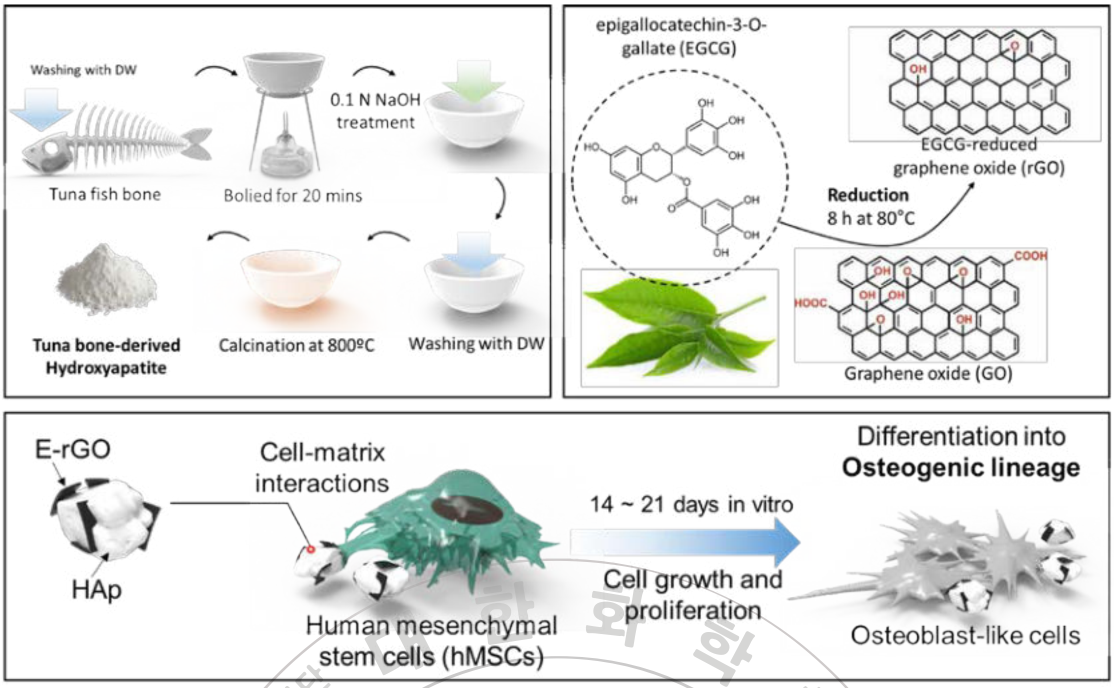
Spontaneous Osteogenic Differentiation of Human Mesenchymal Stem Cells by Tuna Bone-Derived Hydroxyapatite Composites with Green Tea Polyphenol-Reduced Graphene Oxide

Moon Sung Kang, **Dong-Wook Han**[1,*]

Department of Cogno-Mechatronics Engineering, Pusan National University, Korea

[1] *Department of Optics and Mechatronics Engineering, Pusan National University, Korea*

Bone tissue engineering (BTE) has made remarkable progress recently, focusing on enhancing the direct connection between bone and graft to facilitate the healing of damaged bone tissues. A new environmentally friendly and cost-effective method for creating reduced graphene oxide (rGO) and hydroxyapatite (HAp) composites is introduced. These composites, obtained using epigallocatechin-3-O-gallate (EGCG) as a reducing agent and HAp powder from Atlantic bluefin tuna, exhibit exceptional properties for BTE scaffolds with high purity. The study also found that the composites promote the proliferation and early and late osteogenic differentiation of human mesenchymal stem cells (hMSCs). The potential applications of these composites include BTE scaffolds, stem-cell differentiation stimulators, and implantable device components due to their biocompatibility and bioactivity. The research suggests a novel and cost-effective approach to developing environmentally friendly E-rGO/HAp composite materials for BTE applications.


Washing with DW
Tuna fish bone
Bolied for 20 mins
0.1 N NaOH treatment
Washing with DW
Calcination at 800ºC
Tuna bone-derived Hydroxyapatite
epigallocatechin-3-O-gallate (EGCG)
HO
OH
OH
OH
OH
O
OH
OH
OH
EGCG-reduced graphene oxide (rGO)
Reduction
8 h at 80°C
COOH
HOOC
Graphene oxide (GO)
E-rGO
HAp
Cell-matrix interactions
Human mesenchymal stem cells (hMSCs)
14 ~ 21 days in vitro
Cell growth and proliferation
Differentiation into
Osteogenic lineage
Osteoblast-like cells

Poster Presentation : **LIFE.P-54**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Designing Multi-target-directed Flavonoids: A Strategic Approachto Alzheimer’s Disease

Seongmin Park, **Mi Hee Lim**[*]

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

The underlying causes of Alzheimer's disease (AD) remain a mystery, with multiple pathological components, including oxidative stress, acetylcholinesterase, amyloid-β, and metal ions, all playing a role. Here we report a strategic approach to designing flavonoids that can effectively tackle multiple pathological elements involved in AD. Our systematic investigations revealed key structural features for flavonoids to simultaneously target and regulate pathogenic targets. Our findings led to the development of a highly promising flavonoid that exhibits a range of functions, based on a complete structure–activity relationship analysis. Furthermore, our mechanistic studies confirmed that this flavonoid’s versatile reactivities are driven by its redox potential and direct interactions with pathogenic factors. This work highlights the potential of multi-target-directed flavonoids as a novel solution in the fight against AD.

Poster Presentation : **LIFE.P-55**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Impact of sphingosine and acetylsphingosines on the aggregation and toxicity of metal-free and metal-treated amyloid-β

Yelim Yi, Jiyeon Han[1], Hyuck Jin Lee[2], Young S. Park[3], Mi Hee Lim[*]

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

[1]Department of Applied Chemistry, University of Seoul, Korea

[2]Department of Chemistry Education, Kongju National University, Korea

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

Pathophysiological shifts in the cerebral levels of sphingolipids in Alzheimer's disease (AD) patients suggest a link between sphingolipid metabolism and the disease pathology. Sphingosine (SP), a structural backbone of sphingolipids, is an amphiphilic molecule that is able to undergo aggregation into micelles and micellar aggregates. Considering its structural properties and cellular localization, we hypothesized that SP potentially interacts with amyloid-β (Aβ) and metal ions that are found as pathological components in AD-affected brains, with manifesting its reactivity towards metal-free Aβ and metal-bound Aβ (metal–Aβ). In this presentation, we will report that SP is capable of interacting with both Aβ and metal ions and consequently affects the aggregation of metal-free Aβ and metal–Aβ. Moreover, incubation of SP with Aβ in the absence and presence of metal ions results in the aggravation of toxicity induced by metal-free Aβ and metal–Aβ in living cells. As the simplest acyl derivatives of SP, N-acetylsphingosine and 3-O-acetylsphingosine also influence metal-free Aβ and metal–Aβ aggregation to different degrees, compared to SP. Such slight structural modifications of SP neutralize its ability to exacerbate the cytotoxicity triggered by metal-free Aβ and metal–Aβ. Notably, the reactivity of SP and the acetylsphingosines towards metal-free Aβ and metal–Aβ is determined to be dependent on their formation of micelles and micellar aggregates. Our overall studies demonstrate that SP and its derivatives could directly interact with pathological factors in AD and modify their pathogenic properties at

concentrations below and above critical aggregation concentrations.[1]1. Y. Yi, M. H. Lim *et al.*, *Chem. Sci.* 2021, *12*, 2456–2466.

Poster Presentation : **LIFE.P-56**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

NMR Study of the Contribution of the α4 Helix of Human TALE TF, PBX4 to DNA Binding

Youyeon Go, Joon-Hwa Lee[1,*]

Department Chemistry, Gyeongsang National University, Korea

[1]Department of Chemistry, Gyeongsang National University, Korea

Transcription is the first step of gene expression, and RNA polymerase specifically copies a particular part of DNA into mRNA, during which a transcription factor (TF) plays an important role. A TF is a protein family that controls the transcription rate by binding to a specific DNA sequence and thus should contain at least one sequence-specific DNA binding domain. Pre-B-Cell Leukemia Transcription Factor-4 (Pbx4) is a human TF and plays an important role in activating the ephA8 transcription and controlling eye movement. Pbx4 contains a three amino acids loop extension (TALE) homeobox domain (HD) and specifically binds to a common DNA sequence, 5’-TGAT-3’, which was identified by SELEX or random binding site selection. In contrast to MEIS and PREP, PBX proteins have the additional α4 helix at the C-terminal region of the TALE-HD. In order to understand the biological function of the α4 helix during the DNA recognition step, we studied the intermolecular interactions of the TALE-HD of PBX4 including the α4 helix (PBX4-HD) or not (PBX4-ΔCH) with a consensus target DNA duplex using NMR spectroscopy.In this study, we performed heteronuclear single-quantum correlation (HSQC) titrations on complexes of PBX4-HD and PBX4-ΔCH with DNA duplex at various DNA-to-protein molar ratios. We also determined the thermodynamic parameters for DNA binding of PBX4-HD and PBX4-ΔCH using Isothermal titration calorimetry (ITC). This study provides insight into the structural role of the α4 helix of PBX4 protein during its target DNA recognition.

Poster Presentation : **LIFE.P-57**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

NMR Study on target DNA recognition of transcription factor HoxA1

SeungJoon Yu, Hye Bin Ahn[1], Joon-Hwa Lee[2,*]

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

In humans, the Hox genes are distributed into four linkage groups, HoxA, HoxB, HoxC, and HoxD, which locate on chromosomes 7, 17, 12, and 2, respectively. HoxA1 is thought to be involved in the placement of hindbrain segments in the proper location along the anterior-posterior axis during development. Homeodomain (HD) protein has 60 amino acids which are highly conserved in α1 and α3 helices. The N-terminal arm (L1) and loop regions (L2 and L3) between the helices are also well conserved. Interestingly, the second and third residues in L1 loop are conserved as the positive charged residues, Lys(K) or Arg(R), among almost all Hox proteins. However, the HoxA1 has residues Asn(N) and Ala(A) in position 2 and 3 instead of K and R. In order to understand molecular mechanism of DNA recognition of HoxA1, we have performed NMR experiments on the homeodomain of HoxA1 (HoxA1-HD) complexed with 10-bp consensus DNA and 10-bp single variant DNA duplexes, at a variety of DNA-protein molar ratios. In addition, to clarify the role of residues 2 and 3 in Loop 1, we prepared HoxA1-KR mutant in which residues N2 and A3 are replaced by K2 and R3, respectively, and compared its structural feature in a complex with DNA with those of wild-type HoxA1-HD. We also determined the thermodynamic parameters for each DNA binding of WT HoxA1-HD and HoxA1-KR mutant using Isothermal titration calorimetry (ITC). Our study provides an insight into the role of residues N2 and A3 during target DNA recognition of HoxA1.

Poster Presentation : **LIFE.P-58**

Life Chemistry

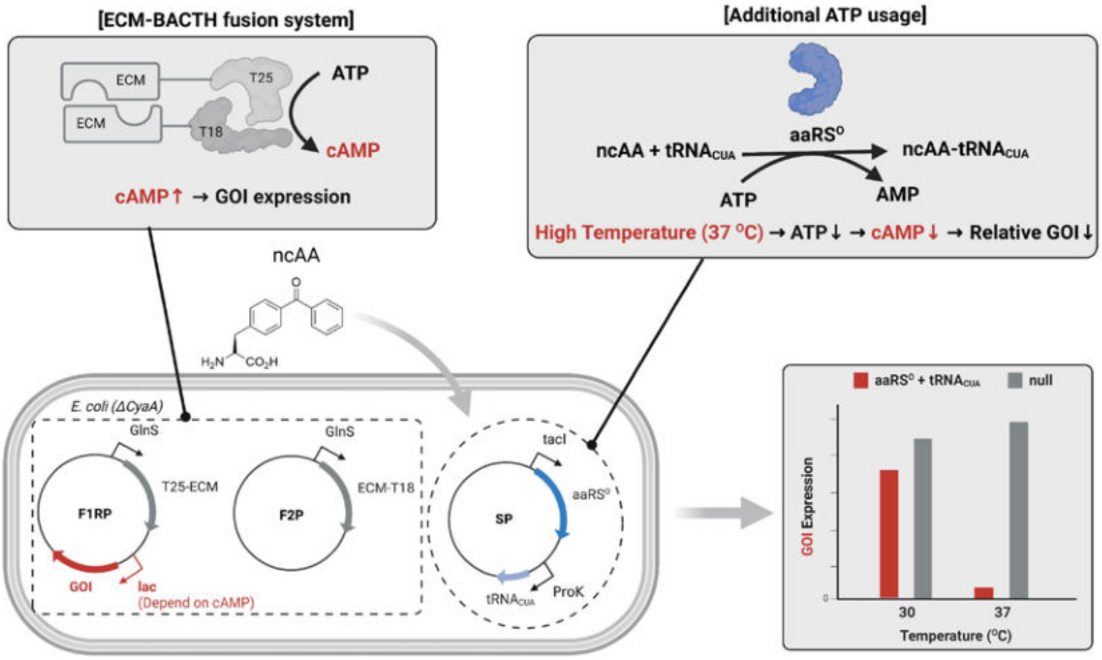
Exhibition Hall C FRI 11:00~13:00

Impact of exogenous aminoacyl-tRNA synthetase and tRNA on temperature sensitivity in *Escherichia coli*

Jongdoo Choi, Ji Yeun Ahn, Minseob Koh[*]

Department of Chemistry, Pusan National University, Korea

Genetic code expansion (GCE) is a powerful tool that expands the genetic code of an organism by incorporating non-canonical amino acids (ncAAs) into proteins using engineered tRNAs and aminoacyl-tRNA synthetases (aaRSs). While GCE has opened up new possibilities for synthetic biology, little is known about the potential side effects of exogenous aaRS/tRNA pairs. In this study, we investigated the impact of exogenous aaRS and amber suppressor tRNA on gene expression in *Escherichia coli*. Our findings show that high consumption of cellular ATP by exogenous aaRS/tRNA at high temperatures leads to a shortage of cAMP, causing temperature sensitivity in the expression of catabolite activator protein-controlled genes in *cyaA* knockout *E. coli*. This temperature sensitivity was observed with exogenous aaRS or tRNA alone, indicating imperfect orthogonality of them. We utilized this temperature sensitivity to construct a dual-input triggered gene expression system in *E. coli*, by fusing a *p*-benzoylphenylalanine dependent variant of *E. coli* chorismite mutates with split subunits of *Bordetella pertussis* adenylate cyclase. Our study provides new insights into the potential side effects of exogenous aaRS/tRNA pairs and offers a new approach for constructing a dual-input triggered gene expression system.


[ECM-BACTH fusion system]
ECM
ECM
T25
T18
ATP
cAMP
cAMP↑ → GOI expression
[Additional ATP usage]
aaRS^{O}
ncAA + tRNA$_{CUA}$
ncAA-tRNA$_{CUA}$
ATP
AMP
High Temperature (37 °C) → ATP↓ → cAMP↓ → Relative GOI↓
ncAA
O
H_2N
CO_2H
E. coli (ΔCyaA)
GlnS
GlnS
T25-ECM
ECM-T18
F1RP
F2P
GOI
lac
(Depend on cAMP)
tacI
aaRS^{O}
SP
tRNA$_{CUA}$
ProK
aaRS^{O} + tRNA$_{CUA}$
null
GOI Expression
0
30
37
Temperature (°C)

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-59**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

Comparison of Z-DNA and Z-RNA binding mode of the ADAR1-Zα protein mutants

Juhee Lim, Joon-Hwa Lee[1,*]

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

The human RNA editing enzyme ADAR1 (double-stranded RNA deaminase I) deaminates adenine in pre-mRNA to yield inosine, which codes as guanine. These A-to-I conversions can lead to functional changes in the resulting proteins. ADAR1 has two left-handed Z-DNA binding domains, Zα and Zβ, at its NH2-terminus and preferentially binds Z-DNA, rather than B-DNA, with high binding affinity. The Zα domains of human ADAR1 bind to Z-DNA via intermolecular interaction mediated by the α3-core and β-hairpin. The substitution of P193, which located in β-hairpin, to A caused Aicardi -Goutières syndrome. In this study, we performed heteronuclear single quantum correlation (HSQC) titrations on complexes of the P193A mutant of ZαADAR1 with DNA or RNA duplexes at various DNA-to-protein molar ratios. According to Previous research of wild type hZαADAR1 demonstrates the unique dynamics of hZαADAR1 during the A−Z transition of RNA, in which the hZαADAR1 protein forms a thermodynamically stable complex with Z-RNA, similar to Z-DNA, but kinetically converts RNA to the Z-form more slowly than DNA. However, this study found that P193A does not bind well to Z-RNA. The same experiment was also performed on T191A, another mutation located in the β-hairpin. The results showed a similar trend to the hZαADAR1. Comparison of these results provides the structural information to explain the origin of Aicardi-Goutières syndrome.

Poster Presentation : **LIFE.P-60**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Genetic encoding of fluorogenic synthetic amino acids for bioimaging

Hwiyeong Lee, Minseob Koh*

Department of Chemistry, Pusan National University, Korea

Genetically encoded fluorescent proteins are pivotal for visualizing proteins and delving into their biological processes. However, the practicality of green fluorescent protein (GFP) derivatives is often hampered by their size (> 20 kDa) and the need for terminal site fusion. To overcome this, we are venturing to create a genetically encoded fluorogenic amino acid (fAA) tailored for bioimaging applications. The genetic code expansion technique facilitates the site-specific incorporation of a synthetic noncanonical amino acid into proteins, ensuring only minimal structural interference with the target protein. Our strategy harnesses an arylideneimidazolinone core, emulating the GFP fluorophore 4-hydroxybenzlidene imidazolinone. We are in the process of crafting arylideneimidazolinonyl homoalanine (termed AIA) derivatives, with an ambition to generate fAAs covering the entire visible color range. As an initiative step, we have synthesized 4-(benzylidene)-1-aminopropanoic acid-2-methyl-5-imidazolinone (AIA-1). Our mass spectrometry findings confirm that AIA-1 can traverse the *E. coli* cell wall and sustain its presence in the cytosol for up to 24 hours. In a viscous medium like glycerol, AIA-1 exhibited fluorescence with peak emissions at 493 nm and 588 nm. Notably, its fluorescence diminished by nearly five-fold in water. For the incorporation of AIA-1 into target proteins in *E. coli*, we employed a selection strategy with the *M. barkeri* pyrrolysyl-tRNA synthetase library. Simultaneously, we are expanding the AIA series, adding diverse substituents to the benzene ring, aiming for a spectrum of electronic features in the fluorophore. Once encoded, the compact size and full-color tunability of the AIA series promise to be invaluable tools for bioimaging.

Poster Presentation : **LIFE.P-61**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

A Microbial Biosensor for Fluoride Ion Detection

Soran Kim, Minseob Koh[1,*]

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

We have devised a microbial biosensor to detect fluoride ions using live *Escherichia coli*. The teoc (2-(trimethylsilyl)ethoxycarbonyl) group serves as a protecting group for amines, and can be cleaved in the presence of a fluoride ion source. One can mask protein function if selective teoc conjugation to the essential lysine residue is achieved. The non-functional masked protein can then be reactivated by environmental fluoride ions. To this end, we synthesized the noncanonical amino acid TeocK by protecting the ε-amino group of lysine with teoc. To introduce TeocK site-specifically, we employed the genetic code expansion strategy. We successfully incorporated TeocK using a variant of the *Methanosarcina barkeri* pyrrolysyl-tRNA synthetase (Y271A and Y349F, TeocKRS) in combination with the *Methanosarcina mazei* tRNA_{CUA} pair in *E. coli*. To determine if the protein incorporating the teoc group can be deprotected by fluoride, we treated it with fluoride ion (NaF, 10 mM) and confirmed partial deprotection (2.12% conversion) using mass spectrometry. We are now attempting to regulate the T7RNA polymerase gene using fluoride ions and enhance the incorporation efficiency (0.90 mg sfGFP-Y151TeocK/L culture) of TeocK by evolving the TeocKRS through continuous directed evolution. Additionally, we synthesized the tyrosine variant noncanonical amino acid DTPY using another fluoride-cleavable protecting group, dimethyl thiophosphinoyl, to conditionally cage the phenolic OH group in tyrosine. Finally, we aim to engineer microbes to be sensitive to environmental fluorides.

Poster Presentation : **LIFE.P-62**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Understanding the DNA recognition mechanism of FOXO4 through NMR investigation

Donghoon Kang, Min June Yang[1], Chin-ju Park[*]

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

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

FOXO4, a member of the FOXO transcription factor family, is a key regulator of gene expression, impacting various cellular functions like cell proliferation, apoptosis, metabolism, and aging. FOXO4 comprises the forkhead DNA-binding domain (FHD) responsible for binding to DNA and the conserved region 3 (CR3) domain utilized for recruiting other transcription factors. However, the precise mechanism by which FOXO4 recognizes specific DNA sequences remains unclear. To explore this, we employed solution NMR techniques including paramagnetic relaxation enhancement, heteronuclear single quantum coherence, and 15N spin relaxation parameters. We analyzed the dynamic properties and identify the specific region of FHD that is influenced by DNA binding. During the interaction between FHD and specific DNA, the CR3 undergoes dissociation from FHD. In contrast, this region still interacts with FHD in the presence of nonspecific DNA. Interestingly, the FHD-DNA complex exhibited distinct differences in exchange modes at physiological salt concentrations, depending on the DNA sequence. We observed contrasting dynamic characteristics between the FHD-nonspecific DNA complex and the FHD-specific DNA complex. Overall, our research provides insights into the FOXO4's DNA recognition mechanism and proposes a model suggesting its role as a transcriptional initiator.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **LIFE.P-63**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of a Peptide Inhibitor of the FOXO4-p53 Interaction Based on the Sequence of p53 Transactivation Domain

Yeji Lim, Donghoon Kang, Chin-ju Park[1,*]

Gwangju Institute of Science and Technology, Korea

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

Forkhead box O4 (FOXO4) is a member of the forkhead transcription factors of the O class involved in various cellular processes such as proliferation, apoptosis, response to oxidative stress, and aging. The tumor suppressor transcription factor p53 regulates DNA repair, cell cycle arrest, and apoptosis. It is known that protein-protein interaction (PPI) of FOXO4-p53 inhibits the pathways leading to apoptosis, thereby inducing the survival of senescence cells and causing many age-related diseases. To disrupt FOXO4-p53 interaction, we developed the peptide inhibitor based on the sequence of p53 transactivation domain (TAD). We performed a fluorescence polarization anisotropy (FPA) competition assay by introducing site-directed Ala mutagenesis into the peptides in order to identify the critical bidnig residues. Through this experiment, we confirmed that the hydrophobic residues of p53 TAD are important for the FOXO4-p53 interaction. We also introduced hydrophobic cell-penetrating peptide (CPP) sequences to facilitate cellular intake, and observed that the inhibitory peptide with hydrophobic CPP could inhibit the binding of p53 to FOXO4 using nuclear magnetic resonance spectroscopy and FPA competition assay. This study will contribute to the development of senolytics, which selectively eliminate senescent cells, through the development of peptide inhibitors targeting the FOXO4-p53 PPI.

Poster Presentation : **LIFE.P-64**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Temperature-sensitive protein-protein Interaction module for gene expression switch

Jiyeun Ahn, Jongdoo Choi[1], Minseob Koh[1,*]

Pusan National University, Korea

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

We designed a temperature-sensitive (TS) protein-protein interaction (PPI) module for gene expression in *Escherichia coli*. This module was developed from an engineered *E. coli* chorismate mutase (ECM) that forms TS homodimers. In *E. coli* Δ*cyaA*, the fusion proteins ECB-T18 and T25-ECB produced cyclic AMP and induced cAMP–CRP (cAMP receptor protein) related gene expression, but only when homodimerization took place. Using the adenylate cyclase two-hybrid system, we confirmed that the TS ECM-dimerization dependent gene expression showed increased activity at 30°C compared to 37°C. This observation led to the development of the TS PPI module. To develop a versatile and direct regulatory system, we fused the TS ECM module with T7 RNA polymerase (T7RNAp). When the TS ECM dimer effectively assembles under specific conditions (30 °C), the T7RNAp-N terminal and T7RNAp-C terminal components attach, driving gene expression. Conversely, under non-permissive condition (37 °C), dimer formation is impeded, preventing the attachment of T7RNAp-N terminal and T7RNAp-C terminal and resulting in suppressed gene expression. This TS module provides the unique advantage of precise transcriptional control, making it valuable for both protein engineering and synthetic biology.Reference1. Karimova, G.; Pidoux, J.; Ullmann, A.; Ladant, D. A bacterial two-hybrid system based on a reconstituted signal transduction pathway. *Proc. Natl. Acad. Sci. U. S. A*. 1998, *95* (10), 5752–5756.2. Koh, M.; Nasertorabi, F.; Han, G. W.; Stevens, R. C.; Schultz, P. G. Generation of an Orthogonal Protein-Protein Interface with a Noncanonical Amino Acid. *J. Am. Chem. Soc*. 2017, *139* (16), 5728–5731.3. Chee, W. K. D.; Yeoh, J. W.; Dao, V. L.; Poh, C. L. Highly Reversible Tunable Thermal-

Repressible Split-T7 RNA Polymerases (Thermal-T7RNAPs) for Dynamic Gene Regulation. *ACS Synth. Biol*. 2022, *11* (2), 921–937.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-65**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Structural basis for the selective methylation of 5-carboxymethoxyuridine in tRNA modification

Jaehun Yoo, Jungwook Kim*

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

Posttranscriptional modifications of tRNA are widely conserved in all domains of life. Especially, those occurring within the anticodon often modulate translational efficiency. Derivatives of 5-hydroxyuridine are specifically found in bacterial tRNA, where 5-methoxyuridine and 5-carboxymethoxyuridine are the major species in Gram-positive and Gram-negative bacteria, respectively. In certain tRNA species, 5-carboxymethoxyuridine can be further methylated by CmoM to form the methyl ester. Here, we present the X-ray crystal structure of Escherichia coli CmoM complexed with tRNASer1, which contains 5-carboxymethoxyuridine at the 5'-end of anticodon (the 34th position of tRNA). The 2.22 Å resolution structure of the enzyme-tRNA complex reveals that both the protein and tRNA undergo local conformational changes around the binding interface. Especially, the hypomodified uracil base is flipped out from the canonical stacked conformation enabling the specific molecular interactions with the enzyme. Moreover, the structure illustrates that the enzyme senses exclusively the anticodon arm region of the substrate tRNA and examines the presence of key determinants, 5-carboxymethoxyuridine at position 34 and guanosine at position 35, offering molecular basis for the discriminatory mechanism against non-cognate tRNAs.

Poster Presentation : **LIFE.P-66**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Human embryonic stem cell factor L1TD1 dissolves ribonucleoprotein condensates

Young-Soo Kwon

Department of Bioconvergence Engineering, Sejong University, Korea

LINE-1 type transposase domain containing 1 (L1TD1) is an RNA binding protein specifically expressed in mammalian embryonic stem cells. Although L1TD1 is required for self-renewal of human embryonic stem cells and cancer cell proliferation, the role of the cytoplasmic RNA binding protein in regulation of RNA metabolism is poorly understood in both physiological and pathological settings. Although L1TD1 is the only known domesticated gene from a LINE-1 (L1) retroelement, the functional legacy of its ancestral protein, ORF1p of L1, and the novelty are yet to be revealed. Here, we determined L1TD1-RNA interactions on a global scale and found that L1TD1 binds L1 RNA and mRNAs localize to high-density ribonucleoprotein (RNP) condensates. Interestingly, L1TD1 enhanced the translation of a subset of mRNAs enriched in the RNP condensates. In HeLa cells, ectopically expressed L1TD1 facilitates the dissolution of stress granules and granules formed by pathological mutations of TDP-43 and FUS. The ability of L1TD1 to dissolve stress granules may provide novel opportunities for treatment of neurodegenerative diseases caused by disturbed stress granule dynamics.

Poster Presentation : **LIFE.P-67**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Transcriptome-wide location analysis of EIF4A3 binding sites reveals interactions with pre-rRNAs and snoRNAs

Young-Soo Kwon

Department of Bioconvergence Engineering, Sejong University, Korea

EIF4A3 is best known as a core component of the exon junction complex consisting of a large number of proteins. The exon junction complex is assembled in a splicing dependent manner and implicated in mRNA splicing, export, localization, translation and nonsense-mediated RNA decay. However, functions other than as a component of the exon junction complex have been reported. To better understand functions of EIF4A3, direct interactions between EIF4A3 and cellular RNAs on a transcriptome scale were surveyed by using CLIP-seq. As expected, EIF4A3 binding sites were concentrated at ~25 nt upstream of splicing sites. In contrast to previous studies, binding to further upstream regions was not readily detectable, suggesting that EIF4A3 does not function as a translation factor. In contrast to previous reports, the majority of CLIP-seq reads mapped in pre-rRNA and snoRNAs. Mapping to pre-rRNA and snoRNAs was most likely to be reflective of authentic interactions on the basis of the paucity of reads mapping to abundant mature rRNAs, tRNAs and snRNAs. The interactions between EIF4A3 and snoRNAs strongly support the previous reports that EIF4A3 plays a role in rRNA biogenesis and explain strong evolutionary conservation of EIF4A3 genes in a variety of eukaryotes ranging from yeast to humans. Comparison of EIF4A3 binding sites with other rRNA biogenesis factors suggests that the EIF4A3 binding profile is similar to that of fibrilin that is the methyltransferase of 2’ hydroxyl group of rRNAs.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-68**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of *In Situ* Click Chemistry Screening Strategy for a Efficient Discovery of Potent Protein Ligands

Minkyung Kim, Hyun-Suk Lim[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

In situ click chemistry is a target-guided synthesis approach where the target protein acts as the biological template. Two (or more) ligands involving azide-alkyne moiety could be brought into close proximity by the target protein and covalently assembled through the cycloaddition. As a result, the highly potent bivalent ligand which is thermodynamically stable and has the most optimized orientation could be developed. These features allow *in situ* click chemistry to be utilized as the attractive screening method. In this study, we have focused on new ideas that increase the library diversity and efficiency over current *in situ* click chemistry screening method. As a novel screening strategy, we introduced nanoDEL(Nano-based DNA-encoded library) technology, recently developed in our group. NanoDELs use the nanoparticles as solid supports to secure huge diversity and DNA as encoding materials.Herein, for the first time, we have developed the screening method based on *in situ* click chemistry using nanoDELs. As a proof-of-concept study, protein tyrosine phosphatase 1B (PTP1B) and its known ligand (Core1) containing alkyne moiety were used. Core1 has low inhibitory activity and selectivity against PTP1B. For increasing the selectivity by targeting peripheral site, peptoid was chosen as library structure. The peptoid nanoDEL involving azide moiety was constructed with 27 million diversity. From the results of screening, peptoid-based hits showed nanomolar level of inhibitory activity and much more improved selectivity against the target, compared to Core1. We anticipate that this newly developed method would be innovative screening tool in the discovery of the potent protein ligands.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-69**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Design, Synthesis, and Screening of DNA-Encoded Libraries of Macrocyclic Peptides and Peptidomimetics.

Jungyeon Kim, Hyun-Suk Lim*

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

Macrocyclic peptides/peptidomimetics have been received a significant interest as a promising class of compounds that offers a great opportunity to discover potent therapeutic candidates. Macrocyclization increases the conformational rigidity of the molecules and minimizes the entropy penalty upon binding to the targets, thereby enhancing the binding affinity. Macrocyclic peptides/peptidomimetics can even engage therapeutic targets that are involved in protein-protein interactions (PPIs), which have rarely been targeted by small molecule drugs, by covering the flat and wide interfaces with their relatively large surfaces. Moreover, macrocyclic peptides exhibit higher proteolytic stability compared to their linear counterparts. Despite their promising properties as therapeutic candidates, technologies for screening of macrocyclic compounds of unnatural peptidomimetics have been rarely reported, while technologies for the discovery of cyclic peptide ligands, such as phage display and mRNA display, are well established.In this study, we describe the design and synthesis of DNA-encoded libraries of macrocyclic peptides/peptidomimetics, including cyclic peptides and bicyclic peptoids. We developed a robust, DNA-compatible synthetic method that afforded DNA-encoded libraries containing 100 million unique macrocyclic compounds with various side chains. Then we performed screening of the synthesized DNA-encoded libraries against target proteins, and identified macrocyclic compounds that strongly bind to the targets. We believe that the DNA-encoded libraries of macrocycles will serve as versatile tools for the discovery of potent ligands of challenging targets, including ones engaged in PPIs.

Poster Presentation : **LIFE.P-70**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

Development of Nanoparticle-Based Encoded Library Technology as a Versatile Tool for Discovery of Potent Protein Ligands

Hee Myeong Wang, Hyun-Suk Lim*

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

DNA-encoded library (DEL) technology has emerged as a powerful selection tool for discovering bioactive molecules. DELs enable the screening of chemical libraries containing up to billions of molecules, leading to the rapid discovery of potent protein ligands. However, conventional DEL method has inherent limitations stemming from the poor solubility of DNA in organic solvents. Due to the insolubility of DNA in most organic solvents, all reactions used for DEL synthesis require aqueous conditions. This significantly restricts the reactivity scope and structural diversity of synthesized compounds. In this study, we have developed an innovative strategy called nanoDEL, where library molecules and coding DNA tags are displayed on the surface of nanoparticles. Notably, nanoparticles are well-dispersed in both aqueous solutions and organic solvents. This characteristic allows the nanoDEL method to utilize well-established reaction conditions without the need to develop DNA-compatible reaction conditions for library synthesis. In addition, unlike conventional DEL synthesis which require laborious purification processes (*e.g.*, HPLC and lyophilization) in each step, nanoDEL technology eliminates the need for purification steps throughout library synthesis by utilizing nanoparticles as solid supports. The potential of the nanoDEL technology in discovering potent ligands against biological targets was successfully validated through affinity-based selections. On-nanoparticle selections yielded highly effective small-molecule inhibitors for a kinase and peptidomimetic inhibitors targeting protein-protein interaction, exhibiting remarkable activities in the nanomolar range.

Poster Presentation : **LIFE.P-71**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Understanding Actin-Microtubule Architecture and Microtubule Bundle Patterns on Crowded Environment and Confinement Condition

Chang Ho Kim, Sang Ho Lee[1], Albertus Ivan Brilian[2], Eunjin Huh[1], Kwanwoo Shin[1,*]

Institute of Biological Interfaces, Sogang University, Korea

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

[2]*Chemistry, Sogang University, Korea*

Microtubules, a form of rigid cylindrical filaments with diameters of 25 nm and lengths of tens micrometers, and actin, a form of flexible single filaments with diameters of 6 nm and actin filaments can be elongate up to many microns in length, are biopolymers 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 with different effects of their own morphological features by the difference diameters and flexibility of biopolymers. For the architecture and interaction of this biopolymers that are actin networks and microtubules bundles, thus researches in cell and in vitro are very hard and complicate. It is also still unclear how architectures and morphologies of actin networks and microtubules bundles are influenced by spatial confinement and crowded components. So, in simplification of “synthetic cell” approaches, we have done the researches about the morphology of architecture of actin-microtubule bundles and the actin-microtubule bundle patterns on spatial confinement and crowded environment without cross linkers. Actin fibers networks were completely formed at Mg ions above 30 ~ 40 mM, which is the critical concentration of Mg ions for the formation of actin fibers networks, but formation of microtubule bundles did not depend significantly on Mg ions concentration. For actin filaments networks, we were able to construct architecture of branched actin networks and linear actin networks according to the concentration of G-actin. The microtubule architecture and bundles pattern showed different morphological changes depending on the gap height between the two cover glasses. The gap height between two glass plates was from 5 μm to 80 μm. Also, the morphology of microtubules bundles showed results that are greatly affected by the crowded environment. In contrast, actin bundle networks showed a confinement effect only at a scale of several microns as in a very small droplet. We plan to study in more depth the interaction between actin bundle architecture and microtubule bundle architecture in the future. These results will provide us some understanding of the influences of spatial confinement and crowded components for formation and interaction of actin and microtubules networks or bundle patterns.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **LIFE.P-72**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

[Withdrawal] Novel Design of Phase Separation Drivers Based on Fluorescent Proteins

YongJun Ha, Da-Eun Hwang, Da-Hyun Koo[1], Yongwon Jung[2], Jeong-Mo Choi[*]

Department of Chemistry, Pusan National University, Korea

[1]*Pusan National University, Korea*

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

Poster Presentation : **LIFE.P-73**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Biochemical study on the FRET efficiency of various fluorescent protein pairs

Yu Jeong Kim, Jae-Won Soh[*]

Department of Chemistry, Inha University, Korea

Fluorescence Resonance Energy Transfer (FRET) occurs when two different fluorophores are positioned close enough together within 10nm that the emission spectrum of one fluorophore overlaps with the absorption spectrum of the other. In this structural arrangement, the energy from the excited state of the donor fluorophore is transferred non-radiatively to the acceptor fluorophore, which then emits light at a longer wavelength. FRET can be used to detect molecular interactions, conformational changes, and distances between molecules at the molecular level. The efficiency of energy transfer depends on the distance between the donor and acceptor molecules. We generated a series of bacterial expression vectors for His-tagged FRET pairs using different fluorescent proteins such as Cerulean, YPet and Cherry. We also generated various FRET pairs in different orders such as YPet-Cherry and Cherry-YPet. Various FRET pair proteins were expressed in BL21(DE3) E. coli strain and purified to homogeneity with nickel column chromatography. We measured fluorescence of various FRET pair proteins using BioTek Synergy HTX Multi-Mode Microplate Reader and Jasco FP-8550 spectrofluorometer. The FRET efficiency of various FRET pair proteins were analyzed for further application to in vitro protein-protein interaction studies.

Poster Presentation : **LIFE.P-74**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Single-molecule evaluation of fluorescent proteins for gene loci observation in live and fixed Escherichia coli

Jung Bae Son, Nam Ki Lee*

Division of Chemistry, Seoul National University, Korea

Fluorescent proteins (FPs) have played an important role in cellular imaging and have been studied in a purified or bulk level. However, advances in microscopy techniques such as super-resolution imaging, single-particle tracking require evaluation of FPs in single-molecule level in living cells. We evaluated the fluorescence intensity and photostability of FP using Tsr protein expressed in living E. coli. Additionally, we examined FPs within a system designed for the observation of specific gene loci in both living and fixed E. coli cells. Chemical fixation of cells is a common procedure for fluorescence microscopy in chemical biology and is believed to cause no artifacts. However, we found that fixation step can change the appearance of phase separation in live cell which would alter the experimental results. This in vivo evaluation provides invaluable information for advanced cellular imaging using FPs for both live and fixed cell.

Poster Presentation : **LIFE.P-75**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

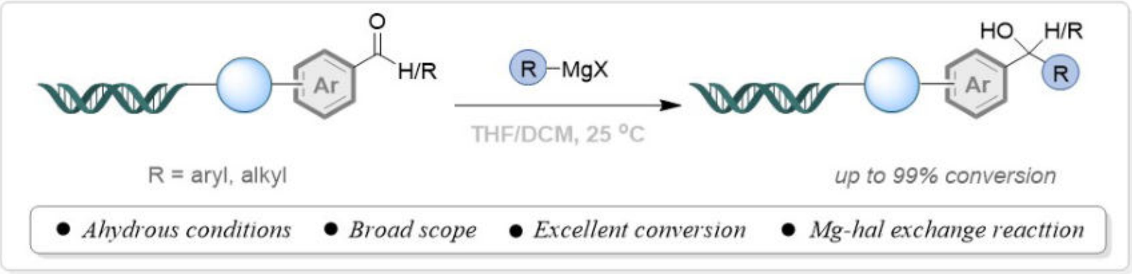
Nanoparticle-promoted on-DNA Grignard reactions for DNA-encoded library synthesis

<u>Muhammad Aliyu Idris</u>[*], Dong Min Shin, Hyun-Suk Lim[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

The hydrophilic nature of dna has curbed the incorporation of many useful anhydrous synthetic methodologies into the existing dna encoded chemical libraries. Hitherto, the Grignard reaction, which is still one of the most powerful coupling tools for carbon-carbon bond formation in organic synthesis, has remained impracticable to conventional dels. This can be attributed to the stringent anhydrous requirement for the reaction, which is inharmonious to the traditional, del setting. Herein, we report the first dna-compatible Grignard reaction using our recently developed nanoDEL procedure by which nanoparticles-support amenable to the Grignard reactions conditions are tactically attached between dna and chemical entity by enzymatic ligation. The protocol possessed good functional group tolerance. The scope was further expanded through on-dna magnesium-halogen exchange reaction. DNA damage assessment using PCR and qPCR analysis showed good retention of dna integrity.



Poster Presentation : **LIFE.P-76**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Investigating the Mode of Action of Antimicrobial Peptoids with Multi-Cationic Side Chains

Yeojin Yun, Jiwon Seo*

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

Peptoids are one of the peptidomimetic materials consisting of an N-substituted glycine backbone and have been utilized for antimicrobial applications. Previously, a cationic amphipathic peptoid with helical conformation, named peptoid 1, showed broad-spectrum antimicrobial activity, but its limited selectivity remained to be improved. In this regard, recent studies have been focused to discover antimicrobial peptoids (AMPeptoids) with enhanced therapeutic windows. Derivatives of peptoid 1 were designed to increase the cationic charge by substituting the *N*Lys residue with multi-cationic residue. The analogs with novel cationic residues generally showed improved selectivity with maintaining antimicrobial activity. In particular, hit peptoid 2 demonstrated negligible hemolytic activity with maintaining minimum inhibitory concentration (MIC) values compared to the control. In this study, we synthesized novel *N*Lys-modified AMPeptoids and the hit peptoid's killing kinetics were compared with colistin that has membrane disrupting mode of action. Due to the difference observed in the kinetic study, we tried to discover its working mechanism through various experiments including membrane disruption, membrane depolarization, reactive oxygen species (ROS) generation analysis, and confocal microscopy. As a result, our study suggests that augmenting cationicity in AMPeptoids can provide a valid strategy to generate a promising antibiotic drug candidate based on peptoid oligomers.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **LIFE.P-77**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

[Withdrawal] Revealing new phosphoarginine binding proteins using chemoproteomic methods

Seungmin Ahn, Jung-Min Kee[*]

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

- Withdrawal -

Poster Presentation : **LIFE.P-78**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of single-cell level bacteria detection and species identification method using super-resolution microscopy

MinJeong Kim, Sung Hun Youn[1], Doory Kim*

Department of Chemistry, Hanyang University, Korea

[1]*LG H&H Ltd., Korea*

The skin's microbiome is believed to have a crucial role in upholding skin health and safeguarding against infections. While most microorganisms residing on the skin are harmless or beneficial, some can lead to skin infections and other health issues. This underscores the significance of identifying and understanding the composition and diversity of skin microorganisms. Nonetheless, conventional diagnostic techniques for assessing the skin's microbiome have limitations in their ability to detect bacteria at low levels and struggle with accuracy. This hampers the early diagnosis of bacterial infections. In this study, we have developed novel methods for detecting and identifying bacterial species with a sensitivity down to the level of individual cells using super-resolution microscopy and AI-based image analysis: a protein quantification-based method and AI-based bacterial image analysis method. We demonstrate that these methods can differentiate between common bacterial members of the skin flora, including Staphylococcus aureus and Staphylococcus epidermidis, and different ribotypes of Cutibacterium acnes, both in purified bacterial samples and in scaling skin samples. The benefits of these techniques, encompassing the absence of time-consuming amplification or purification processes and the sensitivity to detect single cells, facilitate the early identification of bacterial infections. This capability extends even to bacterial samples at a very low concentration, thereby indicating their potential as an advanced platform for the next-generation microbiome detection and single-cell diagnostics.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **LIFE.P-79**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Super-resolution structural study of the crucial roles of extracellular vesicles in host-parasite interactions

Min Jae Kang, Sung Hun Youn[1], Doory Kim[*]

Department of Chemistry, Hanyang University, Korea
[1]*LG H&H Ltd., Korea*

Extracellular vesicles (EVs) have emerged as crucial mediators of intercellular communication in various biological systems. In particular, EVs produced by bacteria exert influence on recipient cells through various aspects, including gene expression, signaling, and pathogenicity. In this study, we investigated the effects of EVs derived from bacteria, on human cells using a stochastic optical reconstruction microscopy (STORM), which is a recently developed super-resolution fluorescence microscopy technique. We utilized STORM to visualize and analyze the interactions of EVs with human cells by observing their ultrastructural changes at a nanometer resolution. Since understanding the impact of EVs on cellular behavior is crucial for unraveling the intricate mechanisms governing human health and disease, this knowledge is expected to pave the way for the development of innovative therapeutic strategies targeting the human microbiome.

Poster Presentation : **LIFE.P-80**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of STRIC (Stimulus TRiggered Cleavage) technology for immune-modulating antibody-payload conjugate

Jeonghyun Lee, Eunha Kim[1,*]

department of molecular science and technology, Ajou University, Korea

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

Based on the human immune system, Activating self-immune cells for the treatment of cancer, known as cancer immunotherapy, have recently hilighted. Especially, immune-modulating antibody-payload conjugate(IMPAC) that conjugate diverse types of payloads with antibodies are being utilized in anticancer therapy or currently undergoing clinical trials. IMAPC generally work by activating immune system. However, in regulating immune activation, it is necessary not only boost the immune activation but also to reduce excessive activity to minimize side effect. Here, we suggest STRIC (stimulus-triggered cleavage) technology, capable of regulating activation using external stimuli (e.g., small molecules). This technology is based on ”click to release” which is the new strategies have been introduced that can be utilized not only for the ligation of two molecules but also for the lysis of bioconjugates to achieve desired functionality. This reaction has found diverse applications within the biological context due to its biocompatibility and rapid response rate. In this study, we are exploring various derivates of the tetrazine core scaffold and apply to STRIC for complement IMAPC.

Poster Presentation : **LIFE.P-81**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Shotgun Scanning Proteomics using Genetically Encoded Photocrosslinkable Amino Acid

Donghyeok Gang, Yeonjin Ko[1,*]

chemistry and biology integtated research center, Korea Institute of Science and Technology, Korea

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

Protein-Protein Interactions (PPIs) play central roles in controlling numerous biophysical and biochemical reactions. Understanding the complex interactions provides fundamentals of life and unveils disease-related factors that could not be identified by genomics or proteomics. Despite the importance and huge interest, current human interactome is quite elusive. This means that current PPI research strategies: immunoprecipitation-based (IP-MS); residue-specific crosslinking-based (RsXL-MS); and proximity affinity labeling-based (PAL-MS), can only provide narrow and shallow information. To address the limitations, we developed and optimized the following two steps: a streamlined method for constructing the amber stop codon (TAG) scanning library and enrichment of interaction partners in residue-scale resolution using site-specifically introduced photocrosslinkable noncanonical amino acid, azibutyl lysine (AbK), via genetic code expansion technology. These methods were applied to detect and analyze interaction partners of KSR2, which is one of the well-known members of the MAPK pathway and also known as the obesity gene. As a result, MEK1, an interacting partner of the KSR2 pseudokinase domain, was successfully detected in a model system. We believe that the high-resolution data from this AbK-based XL-MS (DAzXL-MS) will expand the understanding of protein-protein interaction.

Poster Presentation : **LIFE.P-82**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Porphyrin-Deferoxamine B conjugates for antimicrobial application

Seunghyun Choi, Jiwon Seo*

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

Bacteria secrete siderophores to acquire Fe (III), and theirs iron complexes are transported through the bacterial cell membrane. Linking of an antibiotic drug and a siderophore has been employed as a "Trojan Horse" strategy, which facilitates selective transport of bactericidal agent into pathogenic bacteria via their iron uptake system.In this study, our attempts to synthesize a conjugate of Deferoxamine B (DFO-B), one of the widespread siderophores, and porphyrin as photosensitizer. Three types of photosensitizers are used, meso-tetra(4-N-methylpyridyl)porphine (TMPyP), Pd(II)TMPyP, and tetraphenylporphyrin (TPP), which are known to exhibit photodynamic therapy (PDT) activity. EDC/NHS ester coupling reaction was utilized to form amide linkage. With purified conjugates, biological activity against selected bacteria are being evaluated.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **LIFE.P-83**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of ROS-generating moiety containing peptoid as a potent antimicrobial agent with a multi-target mechanism

Dasom Song, Byeongkwon Kim[1], Yangmee Kim[2,*], Jiwon Seo[*]

Gwangju Institute of Science and Technology, Korea

[1]*Konkuk University, Korea*

[2]*Department of Biotechnology, Konkuk University, Korea*

Antimicrobial peptides (AMPs) have shown promise as potential drugs due to their broad-spectrum activity. To improve their efficacy and selectivity for further development, researchers have utilized peptoids with an abiotic N-substituted glycine backbone to introduce chemical diversity. In this study, the amino terminal Cu(II) and Ni(II) binding (ATCUN) motif was incorporated into antimicrobial peptoids, resulting in complexes capable of generating reactive oxygen species (ROS) upon binding with Cu(II) or Ni(II). The hypothesis was that ROS-induced oxidative damage could enhance the potency of the peptoids. The results demonstrated that the addition of the ATCUN motif increased the hydrophilicity of the peptoids, leading to lower levels of hemolysis compared to the parent peptoids. Mechanism studies revealed that the peptoids caused disruption of bacterial membranes, flocculation of intracellular biomass, oxidation of DNA, and lipid peroxidation. In a mouse model of sepsis induced by Gram-negative bacteria, the ATCUN-peptoid exhibited low toxicity and potent therapeutic efficacy. Overall, this study proposes a strategy to enhance the potency of membrane-targeting antimicrobials by incorporating ATCUN motifs and exploiting oxidative damage as a mechanism for bacterial cell death.

Poster Presentation : **LIFE.P-84**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Observing Nanoscale Deformation of Actin in Human Dermal Fibroblasts using Super-resolution Microscopy

Sang Ho Lee, Albertus Ivan Brilian[1], Chang Ho Kim[2], Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea

[1]*Chemistry, Sogang University, Korea*

[2]*Institute of Biological Interfaces, Sogang University, Korea*

Cytoskeletal proteins provide mechanical tensions within cells that regulate critical cellular functions. While many techniques explored protein deformations on a macroscale, only few focused on the mechanosensing on a nanoscale. Furthermore, a model of actin deformations in mammalian cells due to mechanical stress has not been investigated. To look at series of protein deformations on the mechanosensing on nanoscale, we used super-resolution microscopy and a manual cell stretching device to unidirectionally stretch actin fibers of a human dermal fibroblast until nanoscale deformations were observed. Super-resolution microscopy, stimulated emission depletion microscopy (STED), allowed observing subdiffractional tears that were once unresolved using conventional confocal microscopy, and the elastic deformation of the substrate enabled finding the minimum threshold mechanical force needed to make nanoscale deformations in the adherent cell. Finding the mechanical limitation of cytoskeletal proteins in nanoscale will aid predicting their mechanoresponsive behaviors on a macroscopic level.

Poster Presentation : **LIFE.P-85**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Ultrashort antimicrobial peptoids for improved cell selectivity and drug resistance

Heewoong Yoon, Jiwon Seo*

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

Antimicrobial peptides (AMPs) are promising therapeutics to combat MDR bacterial infections. Colistin, one of the most studied AMP, has been used to treat multidrug-resistant Gram-negative infections as a last-resort treatment, and daptomycin has been approved by the Food and Drug Administration (FDA) for topical infections. Although much attention has been focused on naturally occurring AMPs, most of these native AMPs are not cell selective and can cause severe cytotoxicity for mammalian cells. Ultrashort peptides have attracted considerable interest as an alternative to natural peptides due to their broad-spectrum antimicrobial activity, low cytotoxicity, and advantage of low cost for manufacturing. Herein, we designed and synthesized ultrashort antimicrobial peptoids with *C*-terminus modifications, and evaluated their biological activity. The peptoids exhibited potent antimicrobial activity and enhanced selectivity for bacterial cells. Moreover, the peptoids displayed a low tendency of drug resistance development than conventional antibiotics, such as norfloxacin and colistin. There were differences in biological activity based on the peptoid sequence and the *C*-terminal motif. These results indicate that ultrashort peptoids have strong potential as a new class of novel antibiotic therapeutics.

Poster Presentation : **LIFE.P-86**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Extracellular matrix proteins modify the lipid distribution observed in an artificial cell model

Huong Thanh Nguyen, Kwanwoo Shin[1,*], Sang Ho Lee[1], Chang Ho Kim[2]

Chemistry, Sogang University, Vietnam

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

[2]*Institute of Biological Interfaces, Sogang University, Korea*

Lipid rafts are small regions within the cell's outer membrane, comprised of specific lipids and proteins. Although the existence of these rafts is widely acknowledged, ongoing research focuses on understanding how they form, their size, and structure, leading to various proposed hypotheses and models. Several recent discoveries pinpoint elements affecting lipid distribution on the cell membrane. Besides the well-established interaction between sphingomyelin and cholesterol, facilitated by hydrogen bonds, a diverse range of lipid-protein interactions contribute to raft formation. Some proteins embedded in the cell's membrane show a stronger attraction to cholesterol, while others can form direct bonds with membrane lipids. Additionally, protein size influences raft dimensions. However, the contribution of extracellular matrix (ECM) proteins - interacting with the outer membrane - to lipid raft development remains unanswered. We designed an artificial cell membrane model with simplified components to directly study lipid distribution in response to interactions. Different ECM proteins lead to varied changes in lipid distribution. Generally, binding ECM proteins stabilize lipid regions, reducing their movement when heated. Fluorescence Recovery After Photobleaching (FRAP) measurements partially explain this process by quantifying differences in lipid movement rates between ECM-bound and free domains. This study introduces a new perspective on factors shaping lipid raft formation and properties.

Poster Presentation : **LIFE.P-87**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Hollow-structured Colloidal Quantum Dots for High-Sensitive Biomolecular Detection

Yonghwan Yoo, Jinhyeon Kang, Yongduk Kim[1,*]

Light/Display Convergence R&BD Division, Cheorwon Plasma Research Institute, Korea

[1]*Lighting/Display Convergence R&BD Division, Cheorwon Plasma Research Institute, Korea*

Colloidal quantum dots (CQDs) have recently attracted much attention for bioimaging applications due to their characteristics of narrow half-width maximum (FWHM), easy emission wavelength tuning, high quantum efficiency, and relatively high stability.The use of CQDs for bioimaging applications requires high dispersibility in hydrophilic solvents. For this purpose, it is common to replace hydrophilic ligands or use additives.However, this process causes a sharp decrease in quantum efficiency (QY).Furthermore, silica beads containing CQDs may be used, but in this case, if they become too large, the CQDs have poor dispersibility in a solvent, making it difficult to use them for bioimaging.A molecular spacer was introduced to improve the dispersibility of hollow silica beads containing CQDs and prevent aggregation. The molecular spacer prevents sedimentation by inducing a repulsive force between silica beads containing CQDs and induces bonding between silica beads and CQDs, enabling improvement of PL strength.In conclusion, it is believed that the synthesized hollow structured CQDs can reduce the loss of antigens participating in the detection of biomolecules and induce high detection sensitivity compared to existing CQDs.

Poster Presentation : **LIFE.P-88**

Life Chemistry

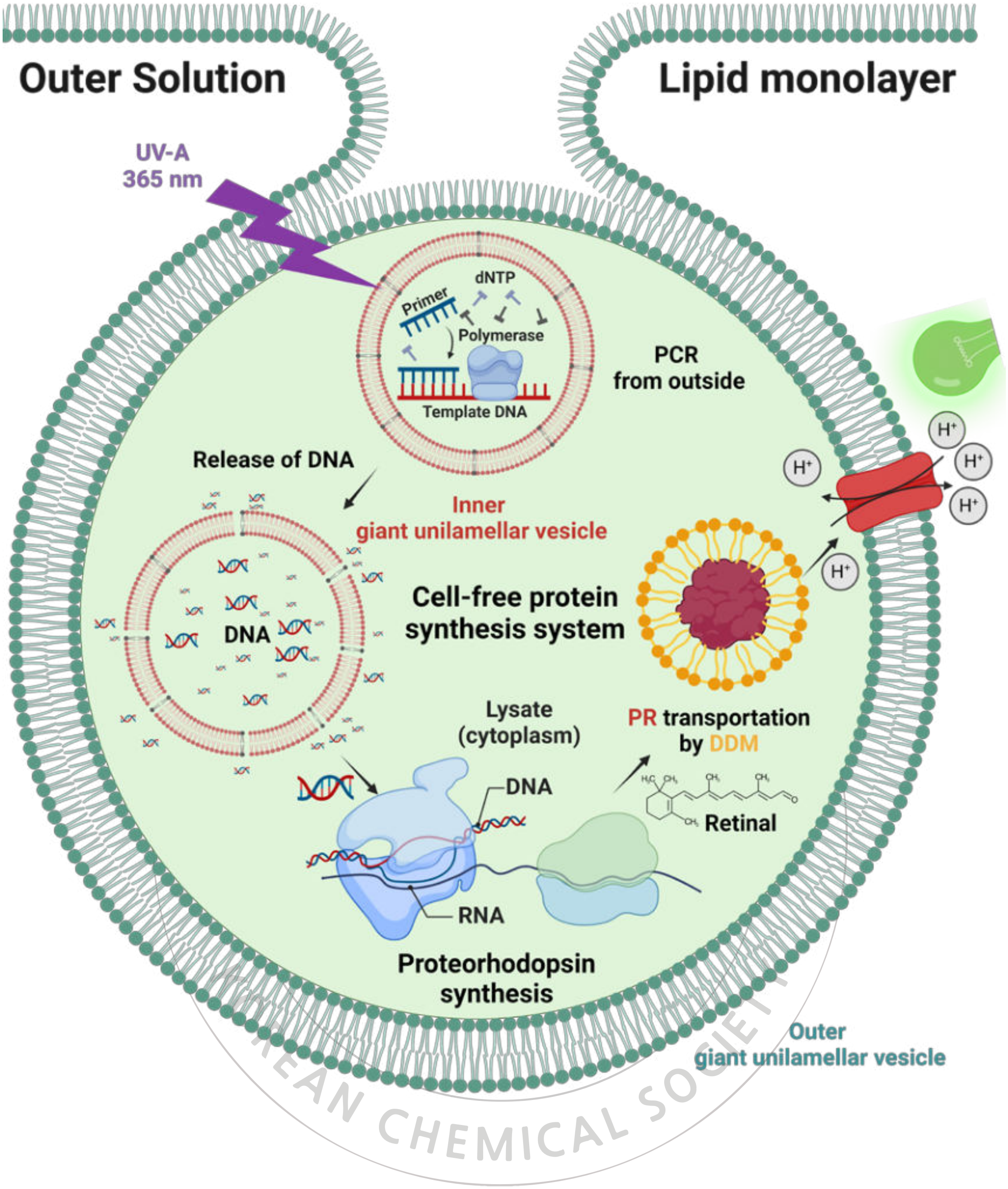
Exhibition Hall C FRI 11:00~13:00

A Controllable Artificial Eukaryotic Cell-like Model

Seangly Tror, Eunjin Huh[1], Huong Thanh Nguyen[2], Kwanwoo Shin[2,*]

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

The term “artificial cell” refers to a wide range of synthetic structures that resemble cells created in the laboratory using various biomolecules and technologies. To investigate biological processes, identify essential molecular parameters in biological systems, and understand the origin of life, researchers have created artificial cells that mimic the structure and function of the living cell. An artificial eukaryotic cell-like structure made of an artificial nucleus that can release plasmid DNA, proteorhodopsin (PR) is synthesized in the cytoplasm, transport proteins to the artificial cell membrane, and function. This model highlights the remarkable ability to regenerate an artificial eukaryotic cell-like model with the same properties, biological activities, and processes as natural cells.Keywords: artificial eukaryotic cell, proteorhodopsin, E. coli, protein transportation


Outer Solution
Lipid monolayer
UV-A
365 nm
Primer
dNTP
Polymerase
Template DNA
PCR
from outside
Release of DNA
Inner
giant unilamellar vesicle
DNA
Cell-free protein
synthesis system
H+
H+
H+
H+
H+
Lysate
(cytoplasm)
PR transportation
by DDM
DNA
Retinal
RNA
Proteorhodopsin
synthesis
Outer
giant unilamellar vesicle

Poster Presentation : **LIFE.P-89**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

Residue 103 is temperature regulation factor in Heat Shock Factor1 trimerization

Bo Hee Choi, Jang-su Park*

Department of Chemistry, Pusan National University, Korea

This study investigated the trimerization mechanism and structure of HSF1 trimerization in humans, goldfish, and pollock at various temperatures. We cloned HSF1 from each of human, goldfish, and pollock wildtypes using PET21b+ vector, proceeded with expression, purification through Ni column, and western blotting through their respective antibodies to investigate trimerization. First, we experimented in the HSF1 DNA-binding domains of humans, goldfish, and pollock, by mutating key residue (103). In addition, it was confirmed that the trimer generation temperature of each species was 42 °C, 37 °C, and 20 °C, respectively. As a result of the mutation experiment, it was confirmed that trimerization occurred at 42 °C when residue 103 was C, 37 °C when it is Y, and 20 °C when it is F, regardless of the species. Also, even if cysteine is present, a trimer is not generated without an aromatic ring such as Y and F. This indicates that, in addition to the previously identified C-C disulfide bonds in humans, C forms a trimer with a new type of bond with aromatic ring residues such as Y and F. Collectively, HSF1 trimer revealed their mechanism of creation through the fact that humans are C-C bonds at 42 °C, goldfish are C-Y bonds at 37 °C, and pollocks are C-F bonds at 20 °C. These results may suggest that the environments in which the three species live are related to their trimer generation mechanisms.

Poster Presentation : **LIFE.P-90**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Cysteine is essential for the HSF1 trimerization.

Chang-ju Lee, Jang-su Park[1,*]

Chemistry, Pusan National University, Korea

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

This study investigated the trimerization mechanism and structure of HSF1 trimerization in humans, goldfish, and walleye pollock at various temperatures. We cloned HSF1 from each of human, goldfish, and pollock wildtypes using PET21b+ vector, proceeded with expression, purification through Ni column, and western blotting through their respective antibodies to investigate trimerization. In previous studies, we confirmed that the residue 103 of HSF1 DNA Binding Domain is a temperature regulation factor. We mutated the 36 residue of human ,goldfish and walleye pollock. First, we experimented in the HSF1 DNA-binding domains of humans, goldfish, and pollock, by mutating key residue 36 that are thought to directly affect trimer generation. As a result of the mutation experiment, it was confirmed that trimerization occurred at 42 °C when residue 103 was C, 37 °C when it is Y, and 20 °C when it is F, regardless of the species. In addition, when mutation of residue 36 was performed, it was confirmed if it had a C at residue 103, the trimer was generated at 42 °C, Y at 37 °C, and F at 20 °C. On the other hand, when there is no cysteine among residues 36 and 103, the results showed that no trimers were generated, even if Y and F are present. This suggests that one or more cysteines are essential for HSF1 trimer production conditions. Also, even if cysteine is present, a trimer is not generated without an aromatic ring such as Y and F. This indicates that, in addition to the previously identified C-C disulfide bonds in humans, C forms a trimer with a new type of bond with aromatic ring residues such as Y and F. Collectively, HSF1 trimer revealed their mechanism of creation through the fact that humans are C-C bonds at 42 °C, goldfish are C-Y bonds at 37 °C, and pollocks are C-F bonds at 20 °C.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-91**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

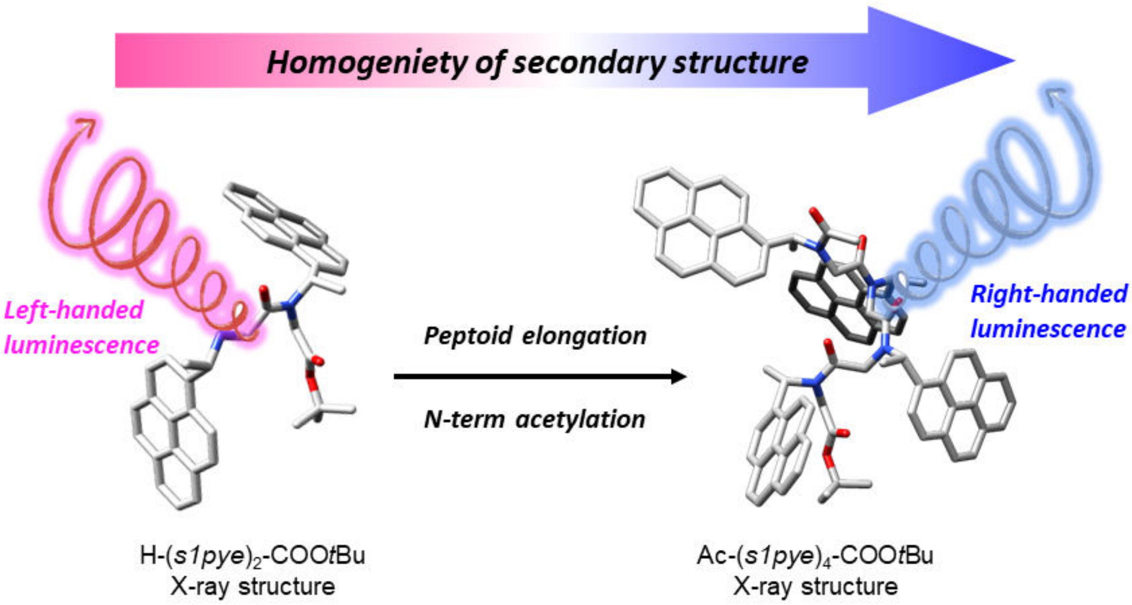
Chiral presentation of pyrene on a peptoid scaffold: secondary structure-driven excimer chirality inversion

Jinyoung Oh, Jiwon Seo[1,*]

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

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

The ability to control the chiral arrangement of chromophores in three-dimensional space is crucial for understanding the relationship between structure and chiroptical properties. Such control enables the prediction of ideal materials for use in chiral photonic applications. In this study, we synthesized and analyzed an optically active multipyrene system on a peptoid helix. We successfully prepared (*S*)-*N*-(1-pyrenylethyl)glycine (*N*s1pye), a pyrene-based chiral submonomer, and incorporated it into various peptoids. NMR spectroscopy revealed a length- and *N*-acetylation-dependent increase in conformational homogeneity in solution, and extreme *cis*-amide stabilization was observed for *N*s1pye. The X-ray crystal structure of the *N*s1pye tetramer revealed a polyproline type-I (PPI)-like helix. All of the pyrene-related absorptions were circular dichroism (CD) active. The CD signal related to the long-axis-polarized transition augmented concomitant with stabilization of the helical conformation. We identified a length requirement of peptoids capable of generating excimers, and significant circularly polarized luminescence (CPL) was observed in the excimer emission region. Pyrene-containing peptoids emitted left-handed CPL in the early stages of elongation. However, as the peptoid acquired a secondary structure in the form of a PPI-like helix, the handedness of CPL became inverted. The determined CPL dissymmetry factor (g_{lum}) was comparable (10^{-2}) to that of chiral organic dyes (10^{-5}–10^{-3}). This new class of helical pyrene–peptoids provides a CPL-active intramolecular excimer, the optical activity of which can be regulated by the homogeneity of the peptoid secondary structure.


Homogeniety of secondary structure
Left-handed luminescence
Right-handed luminescence
Peptoid elongation
N-term acetylation
H-($s1pye$)$_2$-COOtBu
X-ray structure
Ac-($s1pye$)$_4$-COOtBu
X-ray structure

Poster Presentation : **LIFE.P-92**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of fluorescein-labeled iron-chelating peptoid and internalization of the conjugate into gram-negative bacteria

Miram Lim, Jinyoung Oh, Jiwon Seo[1,*]

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

[1]*Gwangju Institute of Science and Technology, Korea*

Iron is an essential nutrient for the growth and survival of many living organisms. Bacteria produce and secrete an organic chelator known as a siderophore to acquire iron under iron-restricted conditions. Siderophore-drug conjugates (aka, sideromycins) can deliver antibiotics across bacterial membrane by the siderophore-mediated iron uptake mechanism and exert bactericidal activity. Cyclic peptoids mimicking bacterial siderophores were developed in our laboratory previously. Among them, a candidate compound exhibited the formation of a hexadentate-coordination geometry with iron (Ⅲ) like ferric enterobactin. We intended to visualize internalization of this siderophore-mimetic peptoid by conjugating it with a fluorescent dye. The carboxyfluorescein (CF) dye was activated primarily using DCC and *N*-hydroxysuccinimide and then coupled with the amine moiety of the peptoid derivative. Confocal imaging demonstrated that the product was internalized into *E. coli* K12. In further studies, we will clarify the uptake mechanisms of these conjugates, which will provide in depth understanding of iron-uptake pathways of bacteria.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-93**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Structural stabilization of dynamic DNA-gold nanoparticle free-standing films via enzymatic ligation

Jong wook Kim[*], **So-Jung Park**[*]

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

Free-standing films of DNA-functionalized gold nanoparticles (GNPs) were fabricated by a combination of layer-by-layer (LbL) self-assembly and plasmonic photothermal patterning [1-3]. Layer-by-layer assembly involves assembling alternating layers of GNPs onto a amino-functionalized glass slide, and plasmonic photothermal patterning utilizes the localized heating generated by plasmonic nanoparticles. To maintain the structural stability of the free-standing films, covalent bonding through DNA T4 ligase is employed in this study. The results show that the enzyme-assisted LbL strategy can generate dynamic nanostructures capable of morphing via various external stimuli, demonstrating how nanotechnology and biomolecular interactions can be harnessed to create functional and adaptable materials.References 1.T. S. Shim, Z. G. Estephan, Z. Qian, J. H. Prosser, S. Y. Lee, D. M. Chenoweth, D. Lee, S. -J. Park and J. C. Crocker, Nat. Nanotechnol. 12, 41 (2016). 2.Z. G. Estephan, Z. Qian, D. Lee, J.C. Crocker and S. -J. Park, Nano Lett. 13, 4449 (2013).3.J. Kim, S. Lee, J. Choi, K. Baek, T. S. Shim, J. K. Hyun and S. –J. Park, Adv. Mater. 34, 2109091 (2022).

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **LIFE.P-94**
Life Chemistry
Exhibition Hall C FRI 11:00~13:00

Investigation of Molecular Mechanisms Underlying Suppressed Aβ42 Aggregation by Small Molecules

Suhyeong Kim, Da Gyeong Hyun, Yeonjeong Kim[1], Jinhui Kim, Gyusub Yoon, Sehyun Hwang[2], Sooyeon Chae, Hugh I. Kim*

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

Alzheimer's disease is the most common neurodegenerative disease characterized by the formation of fibrillar aggregates of amyloidogenic proteins such as amyloid-beta (Aβ) and tau in the central nervous system. These amyloidogenic proteins lack stable structures as they are intrinsically disordered proteins. However, they self-assemble to form intermediates, undergo a transition to a beta-sheet structure, and ultimately lead to the formation of pathogenic fibrillar aggregates. A molecular-level understanding of the mechanisms is important to inhibit the self-assembly of these amyloidogenic proteins.Numerous studies are currently underway to develop therapeutics aimed at inhibiting the self-assembly of amyloidogenic proteins. Small molecules therapeutics offer cost-effective, orally administered options without amyloid-related imaging abnormalities (ARIA). However, small molecule therapeutics that are FDA-approved have not yet been developed. Therefore, to develop effective small molecule therapeutics, the small molecules' molecular-level mechanism inhibiting the amyloidogenic proteins' self-assembly should be investigated.Small molecules that inhibit the self-assembly of amyloid-beta (1-42) (Aβ42) were classified based on their functional groups. We chose promising compounds from each group for higher efficiency. We performed multidisciplinary experiments to evaluate the small molecules' ability to inhibit the self-assembly of Aβ42. Furthermore, in silico molecular docking simulations and molecular dynamics (MD) simulations were conducted to investigate the interactions between the small molecules and Aβ42 and the

structure changes of Aβ42 in the presence of the small molecules. These findings are expected to be crucial in developing small-molecule therapeutics.

Poster Presentation : **LIFE.P-95**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Unveiling the Molecular Mechanism of Amyloid-β (1-42) Aggregation Suppression through Host-Guest Interaction with Cucurbit[7]uril

Da Gyeong Hyun, Suhyeong Kim, Sooyeon Chae, Jinhui Kim, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Amyloid-β (1-42) (Aβ42) is an intrinsically disordered protein (IDP) closely associated with Alzheimer's disease (AD), the most prevalent type of dementia. The inherent self-assembly of Aβ42 triggers the formation of pathogenic amyloid aggregates that accumulate in the extracellular region of neuronal cells, and it becomes a representative hallmark of AD. Cucurbit[7]uril (CB[7]) is a macrocyclic molecule that participates in noncovalent host-guest interactions with diverse guest molecules, composed of seven glycoluril monomers with methylene bridges. CB[7] was widely used for diverse applications including drug delivery and *in vivo* imaging, and it is a potential drug candidate for AD. The suppression ability of CB[7] on Aβ42 aggregation was previously reported (*Angew. Chem. Int. Ed.* 2014, *53*, 7461-7465). However, the underlying mechanism of CB[7] on inhibiting Aβ42 aggregation was not yet precisely demonstrated despite its importance. In this study, we elucidated the molecular-level mechanism of CB[7] suppressing Aβ42 aggregation through structural changes of Aβ42. The structural changes of Aβ42 in the presence of CB[7] were correlated with the high binding affinity of CB[7] with specific amino acids including phenylalanine (Phe) and tyrosine (Tyr). We utilized *in silico* approaches including molecular docking simulations and molecular dynamics (MD) simulations to investigate the interplay between Aβ42 and CB[7]. The outcomes of this research will provide insights into understanding the molecular mechanisms underlying the suppression of Aβ42 aggregation via host-guest chemistry.

Poster Presentation : **LIFE.P-96**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

A Study on the synthesis of organogermanium-vitamin C derivatives and their biological effect

Sangmin Park

Chung-Ang University, Korea

This study proposed the new molecule, which can be used as a functional therapeutic material. The molecule was synthesized using vitamin C as the starting material, which is known to be effective in preventing and improving pigmentation. Despite of highly effective properties, vitamin C is too hydrophilic to penetrate cellular membrane. Thus, lipophilic organogermanium moiety was introduced to vitamin C to increase permeability. And also, organogermanium moiety is known to have good effect on chronic inflammatory skin diseases such as atopic dermatitis. Since antioxidant ability is related to cosmetic effects such as whitening and skin regeneration, DPPH assays is conducted to confirm the efficacy of the molecule as functional material was confirmed in in vitro. In addition, the anti-inflammatory effect was confirmed through an increase in IFN-γ.

Poster Presentation : **LIFE.P-97**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

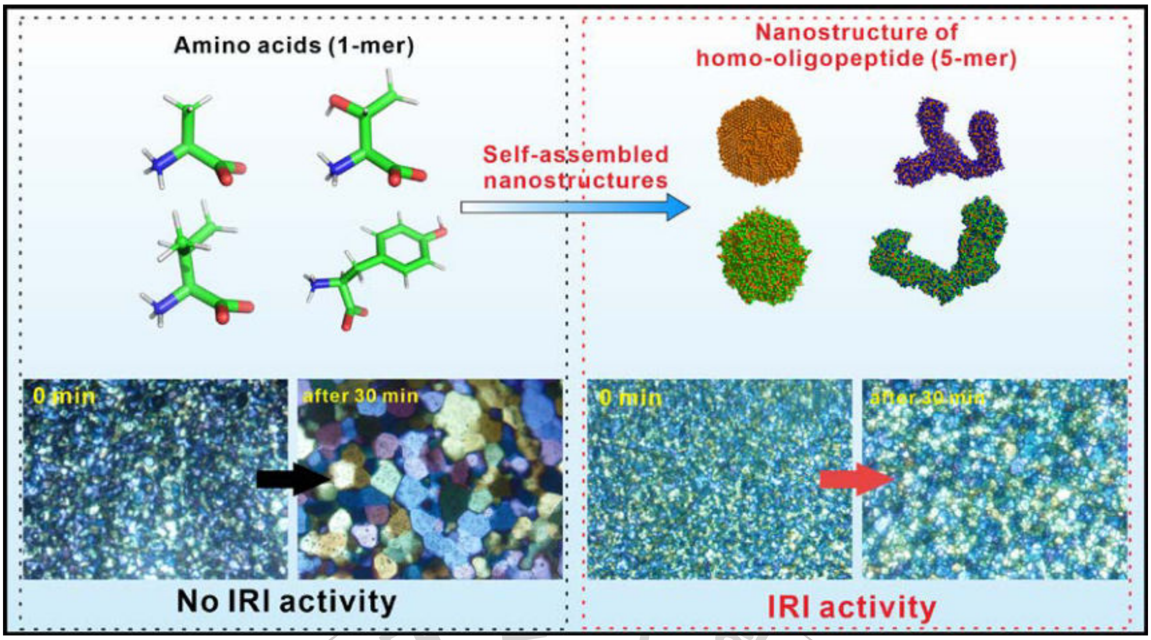
Self-assembled Nanostructure of Homo-oligopeptide with Ice Recrystallization Inhibition Activity

Yong Duk Kim, Dongkwon Lim[1,*]

Korea University, Korea

[1]*KU-KIST Graduate School of Science and Technology, Korea University, Korea*

It is important to mimic the ice recrystallization inhibition activity (IRI) of antifreezing proteins (AFPs) using a variety of materials and nanoscale structures in research that expand the fundamental understanding and future applications of cryopreservation technology. Therefore, it is essential to search for materials with potential IRI activity. Oligopeptide-based materials are promising candidates due to the intrinsic biocompatibility and functionality of the amino acids found in AFPs. This study reports the formation of self-assembled structures using homo-oligopeptides composed of amino acids (e.g., alanine, threonine, valine, and tyrosine) and their resulting morphologies (e.g., spherical, layered and wire structures) in aqueous solutions, and its potential as an ice growth inhibitor. The importance of self-assembled structure formation was confirmed by comparing the IRI activity of solutions containing each amino acid (1-mer) or homo-oligopeptide (5-mer) nanostructure. Among the homo-oligopeptides investigated, the alanine homo-oligopeptide self-assembled structure showed the best IRI activity and low ice nucleation activity. Compared with amino acids, self-assembled homo-peptide nanostructures exhibit superior IRI activity due to their high affinity to ice crystal planes. In the presence of self-assembled homo-oligopeptide nanostructures, they were adsorbed to the ice surface, significantly inhibiting ice growth and increasing hydrogen bond lifetime was confirmed through computer simulation. These results envision excellent performance for self-assembling nanostructures of homo-oligopeptides as desirable and potent inhibitors of ice growth. It can also be used in various fields such as biomedicine and cryobiology


Amino acids (1-mer)
Self-assembled nanostructures
Nanostructure of homo-oligopeptide (5-mer)
0 min
after 30 min
No IRI activity
0 min
after 30 min
IRI activity

Poster Presentation : **LIFE.P-98**

Life Chemistry

Exhibition Hall C FRI 11:00~13:00

Controlling autophagy by spatiotemporal protein photo-oxidation to overcome drug resistance.

<u>Mingyu Park</u>, Jung Seung Nam[1], Taehyun Kim[2], Taiho Park[2,*], Tae-Hyuk Kwon[*]

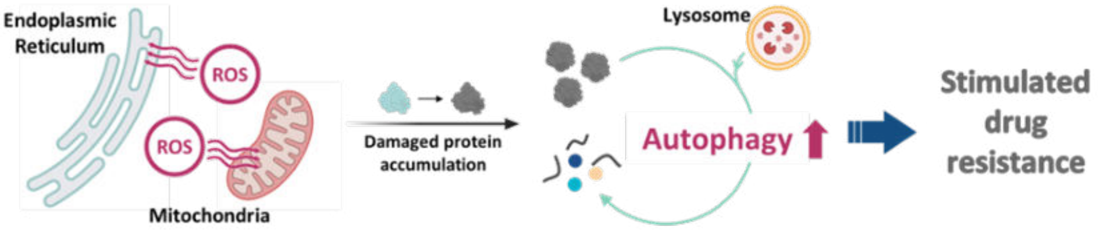
Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

[1]*Department of Genetics and Development, Institute for Cancer Genetics, Department of Genetics and Development, Columbia University Medical Center, New York, NY 10032, USA, United States*

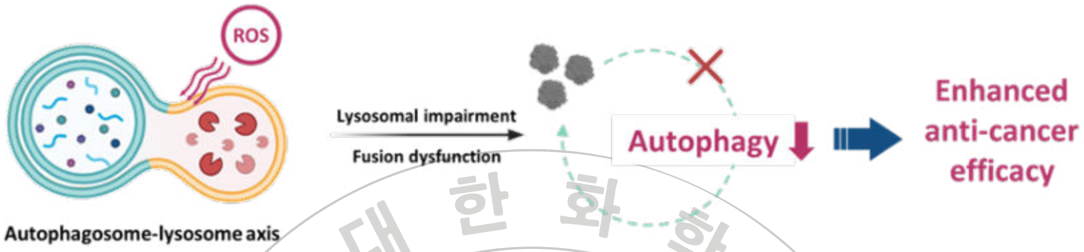
[2]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

Significance: Inhibition of autophagy is an emerging strategy to overcome drug resistance of cancer. However, its photodynamic control has not been clarified since reactive oxygen species (ROS) can either induce or inhibit autophagy. Thus, a rational strategy to perturb autophagy without the activation is required.Approach: To inhibit autophagy, we developed Ir(III) complex B2 that can target and spatiotemporally oxidize lysosome. To study the mechanism of action, we conducted label-free proteomics followed by in vitro experiments for its verification. In vivo efficacy was furter confimed.Results: Our proteomic analysis revealed oxidative modifications at proteins that are responsible for lipogenesis and membrane fusion. Model protein oxidation, confocal microscopy, and immunoblots suggested lysosomal damage, fusion malfunction, and autophagy inhibition. The therapeutic efficacy of the strategy was shown against drug resistant cell lines.Conclusions: This study shows that chemically controlled ROS accumulated at lysosome can successfully inhibit autophagy and suppress drug-resistant cancer.

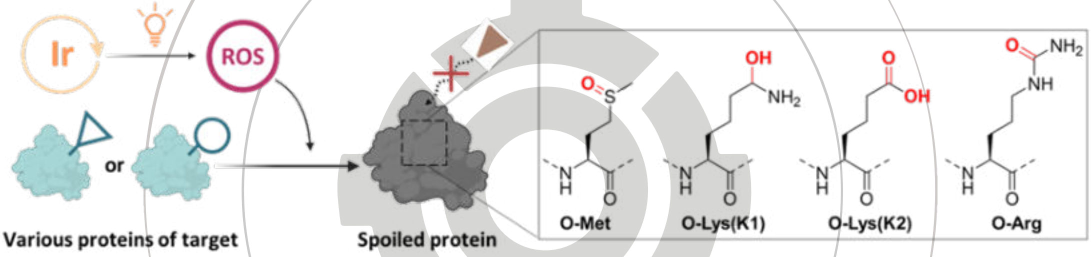
Conventional oxidation targets promote autophagy



Switching target to lysosome can inhibit autophagy



Oxidative modification can circumvent mutation



Poster Presentation : **ORGN.P-99**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

A near-infrared fluorescence chemosensor for selectively detecting hydrazine in aqueous solutions

Jaeseong Kim, **Doo OK Jang**[1,*]

Yonsei University, Korea

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

Hydrazine (N_2H_4) is a strong reducing and highly reactive base. However, it is a toxic inorganic compound that causes liver injury, DNA damage, and even cancer. Therefore, developing a chemosensors for selectively recognizing hydrazine is essential. In this study, we designed a benzothiazole-based near-infrared fluorescence chemosensor with a thioester functional group. The chemosensor recognized hydrazine among biologically relevant chemical analytes and metal cations in a DMF/H_2O (7:3, v/v, pH 7.4) solution. The chemosensor exhibited “turn-on” fluorescence in the near-infrared region at 710 nm with a significant Stokes shift (322 nm). The chemosensor could operate in a range of pH 5–8; the detection limit was calculated to be 5.56 μM. The chemosensor could be applied to detect hydrazine in real water samples.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-100**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Polydomaine-coated agarose film as a template for visible-light-induced polymerization

Ma Hyeonsoo, Hoyun Kim, Jieun Yoon, JungKyu Lee*

Department of Chemistry, Kyungpook National University, Korea

Visible-light-induced radical polymerization has attracted considerable interest in chemobiosensor including colorimetric detection and biomedical engineering, such as tissue engineering, molecular diagnosis, and cell surface engineering. This photoinduced radical polymerization provides excellent reactivity with high spatio–temporal control under mild reaction conditions, including low–energy light, oxygen atmosphere, modest reaction temperature, and water–soluble formulations. Fluorescein and its derivatives act as a photoredox catalyst initiate polymerization of acrylates in the presence of co-initiator (e.g., triethanolamine) with molecular oxygen under the irradiation of visible light. Thus, this polymerization using fluoresceins can amplify the signal of a target analyte (e.g., Hg(II) ions, DNA, protein, cell, and virus) and then apply to the naked-eye detection on a surface such as glass and paper. However, a major drawback of this visible-light photoredox initiation is the necessity of relatively high concentrations of the dye (> 100 nM) used in the photoredox initiating system for a rapid photopolymerization, limiting its practical use in the aforementioned applications. Herein, we employed polydopamine film as a scaffold to enhance the sensitivity of this photopolymerization based signal amplification, and observed significant improvements

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-101**

Organic Chemistry

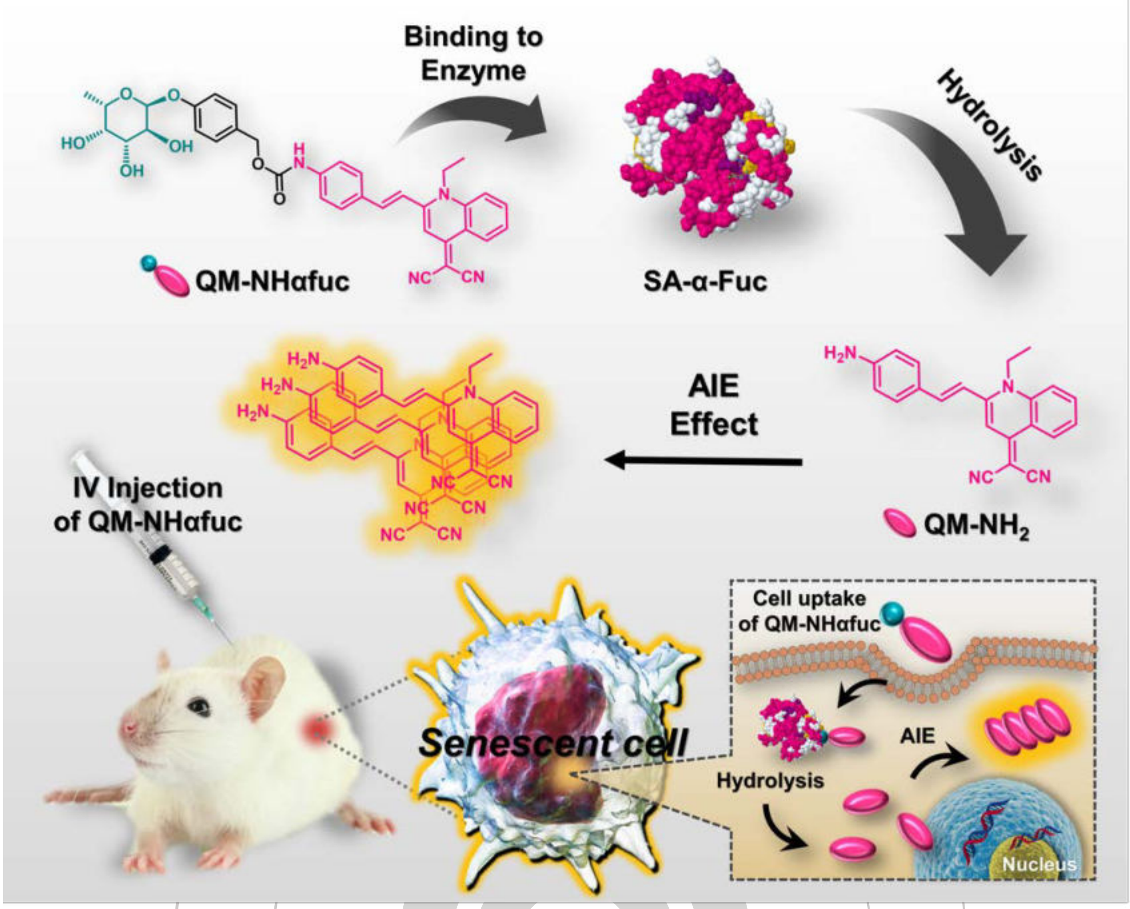
Exhibition Hall C FRI 11:00~13:00

a-L-Fucosidase–responsive AIEgen for cellular senescence in vivo imaging

Miae Won, Jong Seung Kim[*]

R&D institute, TheranoChem Inc., Korea

In vivo sensing of senescent cells is critically important for investigating the senescent process and avoiding its detrimental effects in biological systems. However, current fluorogenic probes for tracing senescent cells heavily rely on a single biomarker, b-galactosidase (b-gal), albeit b-gal is not an absolute biomarker of senescence. Herein, we report an a-L-fucosidase (a-fuc)-responsive aggregation-induced emission (AIE) probe (QM-NHafuc) that enables the detection of senescent cells lacking b-gal. The fidelity of a-fuc as a senescence biomarker was validated in the canonical type of cellular senescence. We also proved that QM-NHafuc serves as the first an-fuc–responsive molecular optical imaging probe capable of detecting cellular senescence both in vitro and in vivo. Notably, we demonstrate that knockdown of a-fuc but not b-gal prevents drug (AZD1152-HQPA)-induced senescence. Our study sheds new insight into the incredible potential of a-fuc as an alternative senescence biomarker of b-gal.


Binding to Enzyme
Hydrolysis
QM-NHαfuc
SA-α-Fuc
AIE Effect
QM-NH$_2$
IV Injection of QM-NHαfuc
Senescent cell
Cell uptake of QM-NHαfuc
Hydrolysis
AIE
Nucleus

Poster Presentation : **ORGN.P-102**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

MoO3 nanoparticle decorated carbon nanotube catalytic application for cross-dehydrogenative coupling-type aza-Henry reaction

Gyuyeong Go, Hyun Chul Choi[1,*]

Department of chemistry, Chonnam National University, Korea

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

Cross-dehydrogenative coupling (CDC) reactions are attracting increasing attention for C−C bond-forming processes. Since it does not require pre-functionalization of the substrates, thus provides an environmentally and economically elegant synthetic routes. Owing to the high dissociation energy of C−H bonds, the CDC reactions are usually catalyzed by transition metal-based materials under appropriate conditions. Herein, we report a new heterogeneous MoO3–carbon nanotube (MoO3–CNT) catalyst, consisting of MoO3 nanoparticles anchored onto a thiol-functionalized CNT substrate by a sol–gel method. We evaluated the applicability of the prepared catalyst in the cross-dehydrogenative coupling-type aza-Henry reaction of N-phenyl-1,2,3,4-tetrahydroisoquinoline with nitromethane. The catalyst showed very good reactivity in aqueous solution.

Poster Presentation : **ORGN.P-103**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Oxygen-Dependent Photoaddition Reactions of Silyl Tether Containing *N*-Phenyl Amino Acid Esters with Fullerene C_{60}.

Suk Hyun Lim, Dae won Cho[*]

Department of Chemistry, Yeungnam University, Korea

The current study investigates SET-promoted photoaddition reactions of silyl tether containing *N*-phenylglycinates and *N*-phenylalaninates, *N*-((trimethylsilyl)methyl)-*N*-phenyl substituted glycinates and alaninates, with fullerene C_{60} to explore how the types of amino acid esters (AAEs) and molecular oxygen affect the photoaddition reaction efficiencies and chemoselectivity of in situ formed radical cations of AAEs. The results showed that under deoxygenated (N_2-purged) conditions, photoreactions of *N*-phenylglycinates with C_{60} produced aminomethyl-1,2-dihydrofullerenes through the addition of alpha-amino radicals arisen by sequential SET and desilylation processes from initially formed secondary anilines to C_{60}. In oxygenated conditions, albeit less efficient, photoreactions of N-phenylglycinates with C_{60} took place to form fulleropyrrolidines through a pathway involving 1,3-dipolar cycloaddition of azomethine ylides to C_{60} assisted by in situ formed $1O_2$. The same types of photoproducts were observed with N-phenylalaninates, though less efficient. The use of methylene blue (MB) as a photosensitizer in the photoreactions under oxygenated conditions was especially effective in enhancing the efficiency of fulleropyrrolidine formation. These results demonstrate that photoaddition reactions of silyl tether-containing *N*-phenyl AAEs with C_{60} can be governed by the reaction conditions and presence/absence of a photosensitizer employed.

Poster Presentation : **ORGN.P-104**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

NHC-Catalyzed Oxidative Cyclization for the Regioselective Synthesis of 3-Aminoisocoumarins

Won Bin Ha, Phil Sik Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

Due to their various biological properties and synthetic utilities in organic synthesis, isocoumarins are one of the most important heterocycles. Therefore, a variety of synthetic methods for their construction have been developed for decades. As part of our continued interest in the NHC-catalyzed oxidative cyclization reaction, we recently developed a new synthetic protocol for the regioselective synthesis of 3-aminoisocoumarins, involving an NHC-catalyzed aerobic oxidation and subsequent cyclization of ynamide-tethered benzaldehydes.

Poster Presentation : **ORGN.P-105**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

NHC/Base-Catalyzed Regioselective Synthesis of (*Z*)-3-Aminomethylenephthalides via Umpolung β-Addition of Ynamides

Phil Sik Kim, Won Bin Ha, So Won Youn*

Department of Chemistry, Hanyang University, Korea

We have successfully developed an NHC-catalyzed lactonization of *o*-ynamidylbenzaldehydes for the regio- and stereoselective synthesis of (*Z*)-3-aminomethylenephthalides. This reaction involves NHC-catalyzed aerobic oxidation of the benzaldehyde moiety followed by base-promoted regioselective cyclization towards the ynamide. This represents the first synthesis of phthalide skeletons through umpolung β-addition of ynamides and the first application of NHC organocatalysis in the context of ynamides. Mechanistic investigations revealed that the extent of proton dissociation of the in situ generated carboxylic acid is crucial for the regioselectivity towards 5-*exo* cyclization, namely β-addition to ynamide.

Poster Presentation : **ORGN.P-106**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Research on the Combination of Urethane Structure and LiFSI for Mitigating Explosion Risks in Lithium-Ion Batteries

Sungjun Park, Wansu Bae[*], Minhyuk Jeon[1,*], Hohyoun Jang[*]

Applied Chemistry, Konkuk University, Korea

[1]*Applied chemistry, Konkuk University, Korea*

Commercially used lithium-ion batteries utilize a liquid electrolyte, including LiPF6, LiFSI, and additives, to improve stability and lifespan. However, relying solely on Li salts in the electrolyte has led to explosions and limited lifespan, prompting extensive research on additives that enhance safety, longevity, and performance. While significant advancements have been made, incidents of explosions still occur, particularly in electric vehicles, and mobile phone batteries experience significant performance degradation within approximately two years.Preventing explosions should be prioritized over performance degradation. In this study, we investigated the combination of fire-resistant urethane structures with LiFSI to mitigate explosion risks in lithium-ion batteries. This approach aims to enhance safety and reliability by reducing electrolyte explosiveness, contributing to the overall improvement of battery systems.

Poster Presentation : **ORGN.P-107**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Hydrophilicity-Driven Predictable Architectures of β-Peptide Foldamers

<u>Yisak Park</u>, Hee-Seung Lee*

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

β-Peptide foldamers, which adopt helical structures analogous to natural α-helices, have garnered attention as notable building blocks. They foster unique, controllable supramolecular architectures with functionalities stemming from their diverse morphologies. In particular, those supramolecular architectures hold the potential for novel functions, distinguishable from natural systems due to the inherent differences between foldamers and their natural counterparts. However, prevailing self-assembly studies have typically modified the component's design or sequence, incorporated additives, or adjusted physicochemical conditions. In this context, we strategically intensified the supramolecular system's complexity in a predictable manner by solely modifying its hydrophilicity. We synthesized a new foldamer by integrating the diethyleneglycol monomethyl ether group while keeping the atom count consistent at the C-terminus of the parent foldamer. As these foldamers do not greatly differ in molecular packing structure, maintaining the same unit cell, they exhibit directional growth when co-assembled with the existing foldamer based on the ratio. This approach offers the potential to pioneer biomimetic materials with designated morphologies.

Poster Presentation : **ORGN.P-108**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Imidazo[1,5a]pyridinylidene-nickel catalysts for acrylate synthesis from ethylene and CO_2

Seyong Kim, Changmuk Kang[1], Huijeong Ryu[2], Wooyong Seong[1], Sukwon Hong[2,*]

Gwangju Institute of Science and Technology, Korea

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

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

Imidazo[1,5-a]pyridine-based N-heterocyclic carbene (ImPy) nickel catalysts were developed for the coupling of ethylene and CO_2 to yield acrylates. Acrylic acid and its derivatives represent valuable chemicals that have been extensively used in the production of superabsorbent polymers, adhesives, coatings, and textiles. While current industrial process for acrylate synthesis involves two-step oxidation of propylene, a direct C-H carboxylation of ethylene with CO_2 has emerged as a more sustainable alternative process. The ImPy-Ni catalytsts were conveniently generated from the corresponding imidazolium salts and commercially available nickel precursors, and exhibited good catalytic activity in the ethylene-CO_2 coupling reaction.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-109**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Visible-light-promoted preparation of sulfonamide derivatives via one-pot reaction of arylazo tetrafluoroborate, DABSO, and benzoyl amine

Truong Giang Luu, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Sulfonamides are one of the most useful pharmaceutical structures due to their significant bioactivities. Therefore, many synthetic techniques of manufacturing sulfonamides have been developed through decades. Recently, the insertion of SO_2 into organic compounds to provide sulfonyl compounds has gained attraction. Particularly in reactions that use light as energy to catalyze the reaction, DABSO has proven to be an effective source of SO_2 suitable for many types of substrates. In this report, we introduce an extremely efficient and practical synthetic processes for preparing sulfonyl amine compounds. This method uses aryldiazo tetraflouroborate salt, DABSO and amino benzoate as starting materials to generate sulfonyl amine compounds under visible light. Studies for this method have demonstrated that various aryldiazo tetrafluoroborate salts and benzoyl amines are suitable substrates. This is promising result to provide useful synthesis of sulfonyl amide structures under mild reaction condition.

Poster Presentation : **ORGN.P-110**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Oxime Esters from Aldehyde via Visible-Light-Induced Multicomponent Reaction

Anh Thu Nguyen, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Oxime esters are an important class of compounds in organic chemistry with many applications. They have been used as reagents or catalysts for the synthesis of various compounds such as amines, amides, esters, and heterocycles. Besides, many bioactive compounds contain oxime ester moieties in their structures. However, the conventional methods to synthesize oxime esters often require two steps: the preparation of oximes from aldehydes or ketones and the esterification of oximes. Herein, a visible-light-induced multicomponent reaction to synthesize oxime esters from aldehydes and N-hydroxyphthalimide (NHPI) esters in one step is reported. In addition, this reaction employed aniline as the nitrogen source and Eosin Y as the photocatalyst. In this study, a variety of oxime esters were successfully synthesized in high yields under mild reaction condition by using this reaction, indicating a potential method for the synthesis of oxime esters.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-111**

Organic Chemistry

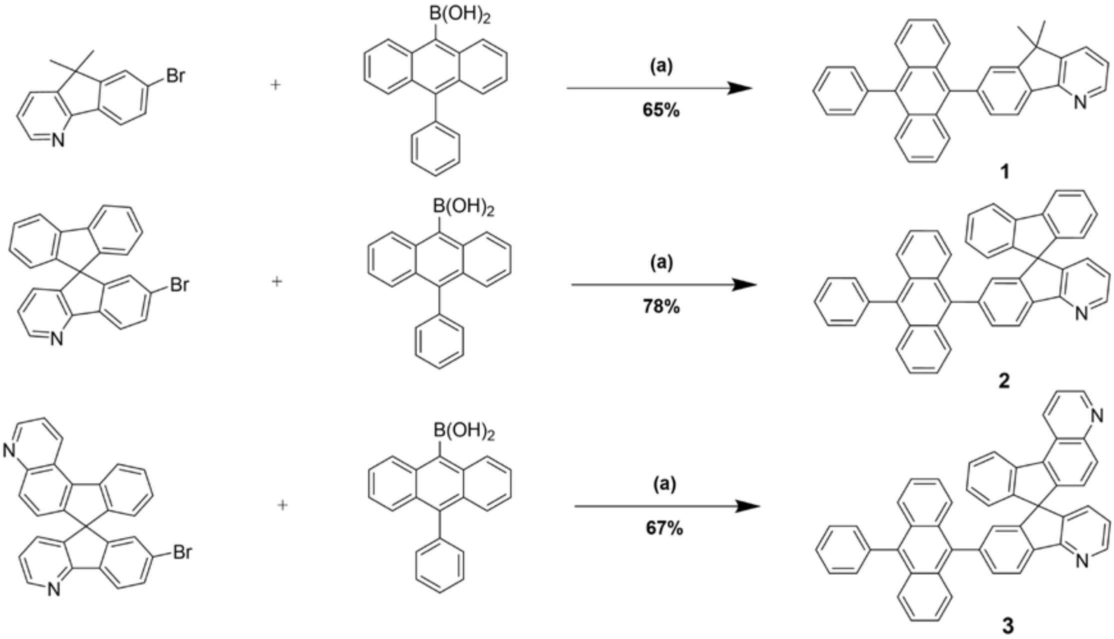
Exhibition Hall C FRI 11:00~13:00

Spirofluorene-Indenopyridine substituted anthracene derivatives for efficient blue Organic Light-Emitting Diodes

Donggun 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, three blue fluorescence materials based on spirofluorene-indenopyridine substituted anthracene derivatives were synthesized and characterized for blue OLEDs. Their photophysical properties have been investigated. To study their electroluminescent properties, OLED devices were fabricated as following sequence: indium-tin-oxide (ITO) (150 nm) / 4,4',4''-Tris[2-naphthyl(phenyl)amino]triphenylamine (2-TNATA) (30 nm) / N,N'-diphenyl-N,N'-(2-napthyl)-(1,1'-phenyl)-4,4'-diamine (NPB) (20 nm) / Blue emitters (20 nm) / bathophenanthroline (Bphen) (30 nm) / lithium quinolate (Liq) (2 nm) / Aluminium (Al) (100 nm). In particularly, a fabricated device using 7'-spiro[fluorene-9,5'-indeno[1,2-b]pyridine] as an emitter exhibited efficient blue emission with the luminous efficiency (LE), power efficiency (PE), and external quantum efficiency (EQE) of 2.96 cd/A, 2.35 lm/W, and 2.50 % at 20 mA/cm-2, respectively, and the CIE coordinates of (0.16, 0.13) at 6.0 V.



Conditions
(a) $Pd(PPh_3)_4$, Na_2CO_3, EtOH and Toluene

Poster Presentation : **ORGN.P-112**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

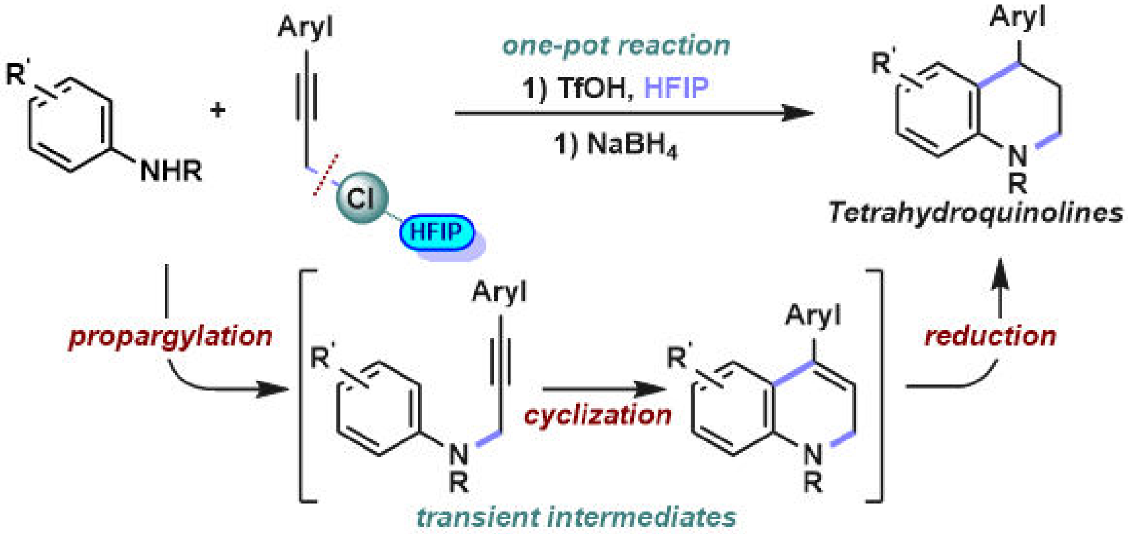
HFIP Empowered Synthesis of C4-Arylated Tetrahydroquinolines with Propargylic Chlorides and Anilines

Seung Hoon Lee, Hyung Min Chi[1,*]

Pohang University of Science and Technology, Korea

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

A practical synthesis of C4-arylated tetrahydroquinolines and quinolones with readily available substrates has been developed. The quinoline framework is constructed by subsequent C-N bond formation and Friedel-Crafts type cyclization. HFIP (1,1,1,3,3,3-hexafluoroisopropanol) serves as a critical component for C-Cl bond activation, which allowed C-N bond formation followed by subsequential acid catalyzed cyclization in one-pot. Resulting disproportionated mixture could be selectively transformed into tetrahydroquinolines by further reduction. To demonstrate the synthetic utilization, total syntheses of aflaquinolone F and I had been accomplished.


Aryl
R'
NHR
+
Cl
HFIP
one-pot reaction
1) TfOH, HFIP
1) NaBH4
Aryl
R'
N
R
Tetrahydroquinolines
propargylation
Aryl
R'
N
R
cyclization
Aryl
R'
N
R
transient intermediates
reduction

Poster Presentation : **ORGN.P-113**

Organic Chemistry

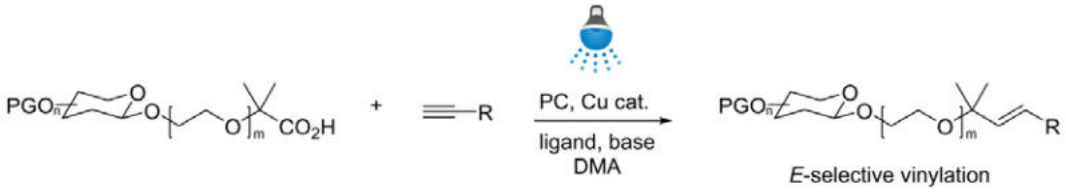
Exhibition Hall C FRI 11:00~13:00

Photoredox Catalyzed Decarboxylative Vinylation of PEG-tethered Sugars and Alkynes

Sang Hyun Park, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

The functionization of saccharides are one of the attractive researches in the field of drug development and biopharmaceuticals. In addition, PEG(polyethyleneglycol) is a polymeric compound with excellent solubility and biosafety, which has been utilized in various applications such as drug delivery, tissue engineering, and biochemical probes. In this work, we present a photoredox catalyzed decarboxylative vinylation of PEG-tethered sugar and alkynes. PEG-tethered sugars can generate alkyl radicals through photocatalyzed decarboxylation, which can then add to alkynes to couple PEG-tethered sugar and alkyne in the presence of a copper co-catalyst. The developed method achieved high E-selectivity in vinylation and tolerated a variety of substrates under mild reaction conditions. This novel approach shows promise as an innovative transformation process for the synthesis of drugs and biochemicals, and is expected to provide new opportunities in the fields of organic chemistry and medicine.



Poster Presentation : **ORGN.P-114**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

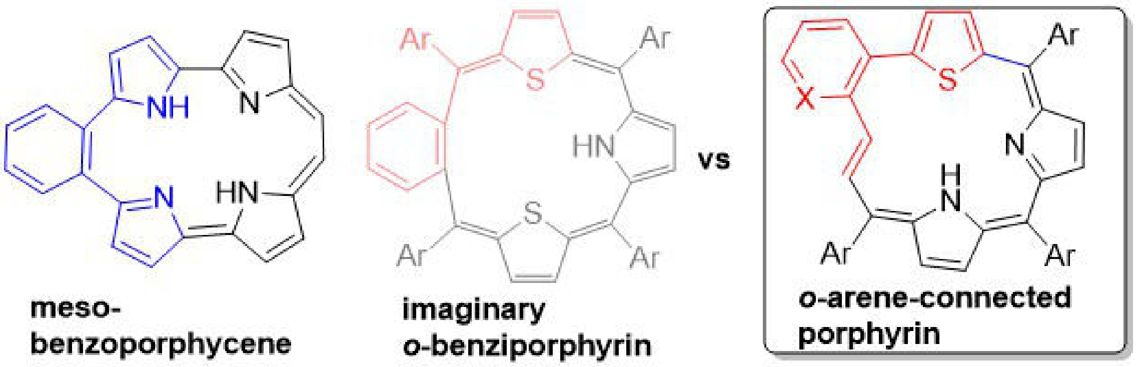
o-(2-Thienyl)vinylarene as an Alternative Synthetic Motif for Porphyrinoids: o-Arene-connected porphyrinoids

Min-Sung Ko, Pradeep Prakash Desale, Dong-gyu Cho[1,*]

Dept. of Chemistry, Inha University, Korea

[1]Department of Chemistry, Inha University, Korea

o-Arene-connected porphyrinoids were synthesized with o-(2-thienyl)vinylarene motif as a new building block for por-phyrinoids. This motif can replace meso-aryl-substituted dipyrromethene and serve as a command key arranging o-connectivity of porphyrinoid. While 6a (benzene version) is very weak, 6b (pyridine version) showed a substantial amount of diatropic ring current due to reduced steric hindrance (without H23) and rigidified Pd-6a became more aro-matic than 6b.



Poster Presentation : **ORGN.P-115**

Organic Chemistry

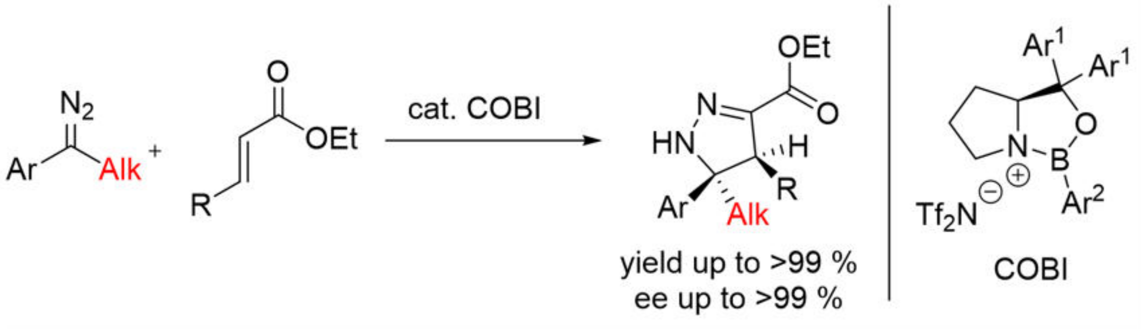
Exhibition Hall C FRI 11:00~13:00

Exploration of Unstabilized Aryldiazoalkanes in Lewis Acid Catalyzed Enantioselective 1,3-Dipolar Cycloaddition

Terim Seo, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Aryldiazoalkanes, especially in the form of diazo compounds, exhibit remarkable reactivity in various chemical transformations such as cyclopropanations and insertions. As a result, they have attracted considerable attention over the past few decades. While aryldiazoalkanes have found widespread application in enantioselective reactions, the exploration of unstabilized aryldiazoalkanes continues to present significant challenges. Herein, our research group has successfully introduced a novel application of unstabilized aryldiazoalkanes in catalytic enantioselective 1,3-dipolar cycloadditions, yielding enantioenriched 2-pyrazolines in excellent yields (up to >99%) with excellent enantioselectivities (up to >99%) using a chiral oxazaborolidinium ion (COBI) catalyst.



Poster Presentation : **ORGN.P-116**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Total synthesis of (E)-Secobutanolides: Structure Analysis of (+)-Litseakolide F and G

Jin Won Lee, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Butanolides and Secobutanolides from the Lauraceae family are prominent γ-lactones and their derivatives respectively, often employed in traditional Chinese and Taiwanese medicine. Compounds characterized by a chiral β-hydroxyl group and a β-branched Morita-Baylis-Hillman (MBH) ester core are of special interest due to their potential in various therapeutic applications, including anticancer and antibacterial properties. Although the stereochemistry of Secobutanolide series and Litseakolide F & G remains elusive, we previously unveiled a high-yielding, enantioselective coupling reaction catalyzed by chiral oxazaborolidinium ion (COBI). Building on this, we introduce a synthetic strategy, leveraging Z→E isomerization, for creating (E)-stereoselective MBH esters, pivotal for crafting chiral (E)-Secobutanolide natural products. This methodology facilitated the total synthesis of the chiral Secobutanolide series and Litseakolide F & G, also permitting the refinement of the structures of the natural products (+)-Litseakolide F and G.

Poster Presentation : **ORGN.P-117**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Dia- and Enantioselective Cyclization reaction of Aryl Glyoxals with Allylsilanes Using Chiral Oxazaborolidinium Ion Catalyst

Dong Kyu Kim, Terim Seo, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Allylsilanes, which are key intermediates in organic synthesis, have been traditionally associated with regio- and stereoselective carbon-carbon bond formation, particularly with carbonyl groups. While the allylation reactions involving allylsilanes with carbonyl compounds like aldehydes and ketones (as demonstrated by the Hosomi-Sakurai reaction) have undergone thorough examination, only a limited number of studies have explored the cyclization reaction of allylsilanes with the aim of constructing carbocyclic and heterocyclic ring systems. Moreover, there has been no previous research that has devised a method capable of simultaneously controlling both diastereoselectivity and enantioselectivity in cyclization reactions. Herein we developed enantioselective cyclization reaction of allylsilanes with aryl glyoxals, employing a chiral oxazaborolidinium ion (COBI) as a Lewis acid catalyst. This innovative method provided tetrahydrofurans achieving high yields (up to 87%) and excellent enantioselectivities (up to >99%).

Poster Presentation : **ORGN.P-118**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Catalytic Asymmetric Formal C–C Bond Insertion of Diazo Compound for the Enantioselective Formation of All-carbon Quaternary Stereocenters

Hye-Min Jeong, Jin Won Lee, Dong Kyu Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Enantioselective synthesis in organic chemistry has evolved to address complex challenges, particularly the creation of all-carbon quaternary stereocenters. Notably, there have been no reports of catalytic asymmetric C–C bond insertion reactions leading to all-carbon quaternary stereocenters containing three carbonyl groups.This reaction pathway produces *β*-keto esters with *α*-quaternary carbon centers and achieves high enantioselectivities (up to 99% ee) and yields (up to 97%). A possible mechanistic explanation supported by Density Functional Theory (DFT) calculations supports the observation of chemoselectivity and stereochemistry. Remarkable for their electrophilic and nucleophilic properties, *β*-keto esters play an important role in synthetic chemistry. The versatile nature of this reaction suggests its potential application in various complex chemical transformations and the synthesis of complex medicinal intermediates.

Poster Presentation : **ORGN.P-119**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

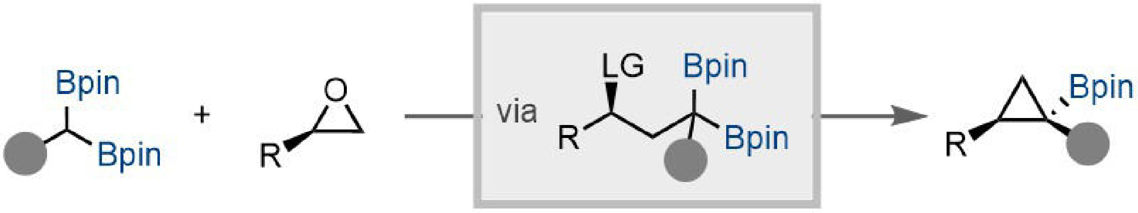
Conversion of Chiral Epoxides with gem-Diborylalkanes: Stereospecific Approach of Secondary and Tertiary Cyclopropylboronates

Gwanggyun Kim, Seung Hwan Cho[1,*]

Department of chemistry, POSTECH, Korea

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

Enantioenriched cyclopropylboronates play a crucial role as key intermediates in the synthesis of various natural compounds and pharmaceuticals containing cyclopropyl groups. Consequently, significant efforts have been dedicated to devising strategies for synthesizing these enantioenriched cyclopropylboronates. However, most of the existing approaches have primarily focused on producing enantioenriched secondary cyclopropylboronates, leaving the synthesis of enantioenriched tertiary cyclopropylboronates relatively unexplored. Herein, we describe the process of converting chiral epoxides utilizing gem-diborylalkane into both secondary and tertiary cyclopropylboronates under transition-metal-free conditions. Our approach unfolds through a three-step sequence: initiation involves the addition of (gem-diborylalkyl)lithium generated from gem-diborylalkanes to chiral epoxides, followed by the introduction of a leaving group and a stereoselective deborylative cyclization, leading to the generation of enantioenriched cyclopropylboronates. Moreover, we showcase additional synthetic modifications that can be performed using the resultant enantioenriched cyclopropylboronates.



- readily accessible reagents
- broad scope
- high diastereoselectivity and enantioselectivity

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-120**

Organic Chemistry

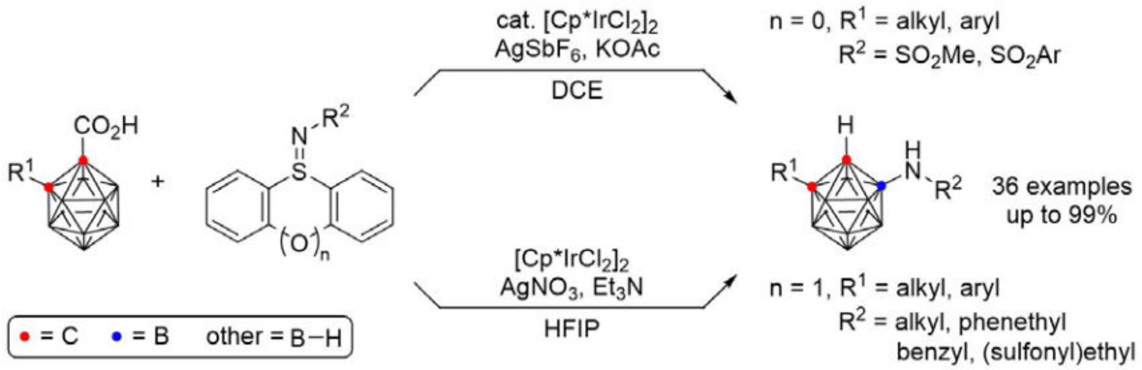
Exhibition Hall C FRI 11:00~13:00

Ir(III)-Catalyzed Regioselective B(4)–H Amination of *o*-Carboranes with Sulfilimines

Park Kyeongna, **Phil Ho Lee***

Department of Chemistry, Kangwon National University, Korea

Because carboranes as a kind of the polyhedral boron clusters have remarkable properties like 3D σ-aromaticity, inherent robustness, and spherical geometry, they have been extensively used in a number of areas including medicines, catalysts, organometallic coordination chemistry, supramolecular design, and optoelectronics. For that reason, an efficient introduction of various functional groups onto the carborane skeleton is required to further expand these applications. Regardless of recent progress for the functionalization of *o*-carboranes, development of a new synthetic method for B−N bond formation on carborane has been a continuing challenge as nitrogen-substituted carboranyl amino acids and nucleosides have been applied as pharmaceutical agents for tumor therapy in boron neutron capture therapy (BNCT). Therefore, regioselective setting nitrogen functional group on carboranes using a variety of nitrogen sources is important. Iridium(III)-catalyzed regioselective B(4)−H amination is developed from the reaction of *o*-carborane acids with sulfilimines without any oxidants under mild conditions, leading to a wide range of B(4)−H aminated *o*-carboranes in good yields with a broad substrate scope. Moreover, the selective B(3,6)-diamination reaction of *o*-carborane acid was achieved. The present reaction is attractive from the practical point of view as dibenzothiophene is quantitatively recovered and reused.


CO$_2$H
R^1
+
N
R^2
S
(O)$_n$
● = C ● = B other = B–H
cat. [Cp*IrCl$_2$]$_2$
AgSbF$_6$, KOAc
DCE
[Cp*IrCl$_2$]$_2$
AgNO$_3$, Et$_3$N
HFIP
n = 0, R^1 = alkyl, aryl
R^2 = SO$_2$Me, SO$_2$Ar
H
H
N
R^1
R^2
36 examples
up to 99%
n = 1, R^1 = alkyl, aryl
R^2 = alkyl, phenethyl
benzyl, (sulfonyl)ethyl

Poster Presentation : **ORGN.P-121**

Organic Chemistry

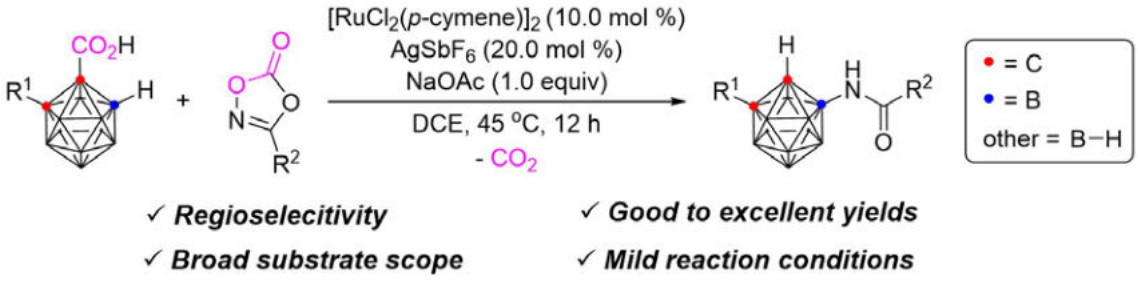
Exhibition Hall C FRI 11:00~13:00

Ru(II)-Catalyzed Selective B(4)–H Amidation of *o*-Carboranes with Dioxazolones

Sugyeong Yoon, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

A ruthenium-catalyzed selective B4 amidation of *o*-carboranes with a variety of alkyl-, aryl-, and heteroaryl-substituted dioxazolones is developed by carboxylic acid-assisted B(4)-H bond activation in *o*-carborane acids, affording a multitude of B(4)-amidated *o*-carboranes in good yields with the evolution of carbon dioxide. In addition, the two-fold selective decarboxylative amidation reaction of the cage B(4)-H bond in *o*-carborane was accomplished.



132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-122**

Organic Chemistry

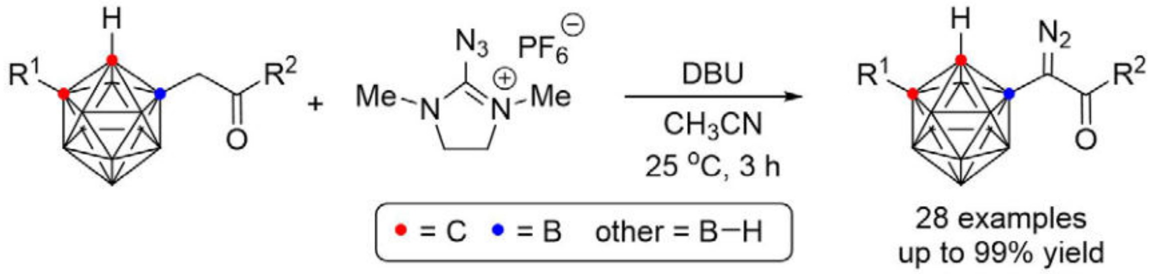
Exhibition Hall C FRI 11:00~13:00

Synthesis of *o*-Carboranyl Diazo Compounds from B(4)-Acylmethyl Carboranes and 2-Azido-1,3-Dimethylimidazolinium Hexafluorophosphate

Eunseo Lee, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

In the diverse area of organic synthesis, diazo compounds have been regarded as amphiphilic reagents owing to their remarkable potential to undertake electrophilic as well as nucleophilic reactions. Hence, the carbon atom of diazo compounds is ideally reacted with electrophiles, whereas the terminal nitrogen atom is tending to be reacted with nucleophiles. Also, diazo compounds can also undergo [3 + 2] cycloaddition reactions, producing diazo moiety-incorporated products. Our studies directed toward the development of synthetic approach using *o*-carborane and diazo compounds and on the basis of recently reported functionalization of *o*-carborane, we described herein an efficient synthetic method for a wide range of *o*-carboranyl-acyl-substituted diazo compounds from the reaction of B(4)-acylmethyl *o*-carborane with 2-azido-1,3-dimethylimidazolinium hexafluorophosphate (ADMP) in good to excellent yields with good functional group tolerance under mild conditions.



☑ ***o-carboranyl-acyl-substituted diazo compounds***

☑ ***mild conditions***

☑ ***good to excellent yield***

☑ ***good functioal group tolerance***

Poster Presentation : **ORGN.P-123**

Organic Chemistry

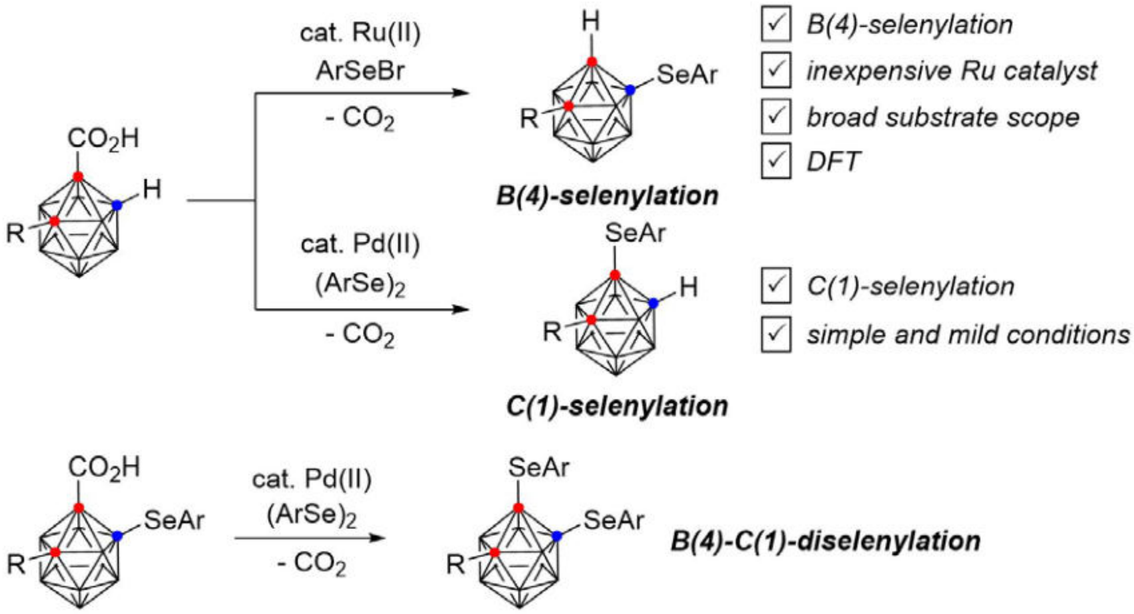
Exhibition Hall C FRI 11:00~13:00

Ru-Catalyzed B(4)-Selenylation and Pd-Catalyzed C(1)-Selenylation of *o*-Carboranes

Yurim Park, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Regiodivergent transition metal-catalyzed B(4)- and C(1)-selenylation reactions of o-carboranes have been demonstrated. Namely, Ru(II)-catalysis selectively generated B(4)-selenylated *o*-carboranes from the reaction of *o*-carborane acids with arylselenyl bromides with the release of carbon dioxide. In contrast, Pd(II) catalysis provided exclusively C(1)-selenylated *o*-carboranes from the decarboxylative reaction of *o*-carborane acids with diaryl diselenides. In contrast to previous milestones in this area, these reactions demonstrate broad substrate scope with excellent yields. Combination of these methods leads to the formation of B(4)–C(1)-diselenylated *o*-carboranes. DFT studies revealed the mechanism of the Ru-process, with initial selenylation of the carborane cluster discovered to be essential for an energetically reasonable decarboxylation. This results in selenylation on the B(4) position prior to the decarboxylation event at C(1). This contrasted with the Pd-process in which the ready decarboxylation at C(1) leads to selenylation at C(1).


cat. Ru(II)
ArSeBr
- CO$_2$
CO$_2$H
H
R
SeAr
B(4)-selenylation
☑ B(4)-selenylation
☑ inexpensive Ru catalyst
☑ broad substrate scope
☑ DFT
cat. Pd(II)
(ArSe)$_2$
- CO$_2$
SeAr
H
R
C(1)-selenylation
☑ C(1)-selenylation
☑ simple and mild conditions
CO$_2$H
SeAr
R
cat. Pd(II)
(ArSe)$_2$
- CO$_2$
SeAr
SeAr
R
B(4)-C(1)-diselenylation

Poster Presentation : **ORGN.P-124**

Organic Chemistry

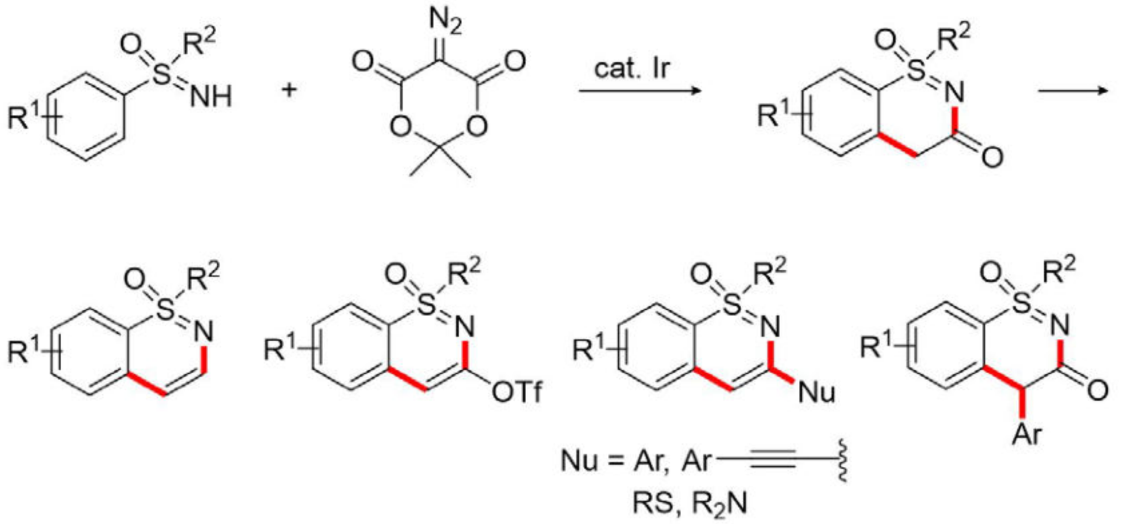
Exhibition Hall C FRI 11:00~13:00

Iridium(III)-Catalyzed C–H Cyclization of Sulfoximines with Diazo Meldrum's Acids for the Synthesis of Cyclic Sulfoximines

Hyeonmi Cho, **Phil Ho Lee***

Department of Chemistry, Kangwon National University, Korea

Iridium(III)-catalyzed C−H cyclization of sulfoximines with diazo Meldrum's acid provided cyclic sulfoximines with a carbonyl group in good to excellent yields. These compounds were easily converted into unsubstituted and arylated sulfoximines. Moreover, the vinyl triflates obtained from the cyclic sulfoximines underwent palladium(II)-catalyzed cross-coupling reactions with a variety of aryl, arylalkynyl, and heteroatom (N and S) nucleophiles, affording a wide range of monosubstituted sulfoximines in high yields.



☑ ***new scaffolds*** ☑ ***low loading of catalyst*** ☑ ***unsubstituted sulfoximine***

☑ ***mono-substituted sulfoximine*** ☑ ***wide functional group tolerance***

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-125**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Microcrystal Electron Diffraction in Determining Crystal Structures of Metal-Biomolecule Complexes

Jaewook Kim, **Hee-Seung Lee***

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

Microcrystal electron diffraction (MicroED) is a cutting-edge crystallographic technique that utilizes electron beams from Cryogenic Electron Microscopy (Cryo-EM) to determine structures of submicrometer-sized crystals. Recent advancements have elucidated crystal structures of small molecules and membrane proteins previously unsuitable for Single Crystal X-Ray Diffraction (SC-XRD). This study successfully determined a crystal structure of a coordination complex formed between an unnatural cyclic β-amino acid and copper bromide using MicroED. The crystals, with a needle-like shape approximately 500 nm diameter, were ideal for MicroED analysis. The resulting diffraction pattern revealed sharp Bragg peaks with a sub-Angstrom resolution. The superior quality of the diffraction dataset allowed for the structure to be solved using ab initio methods. This underscores the immense potential of MicroED in determining the crystal structures of metal-biomolecule complexes, even without prior structural information.

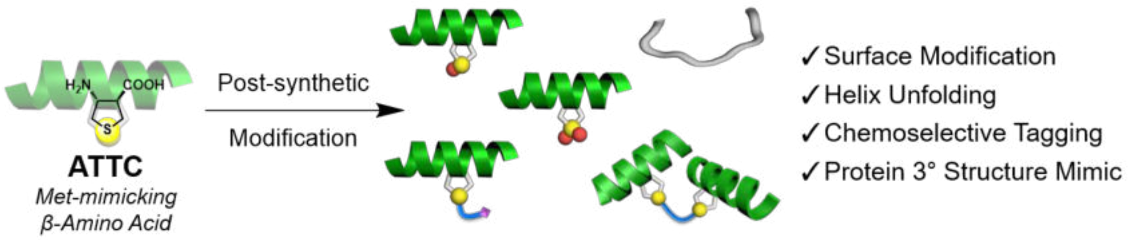
Poster Presentation : **ORGN.P-126**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Cyclic β-Amino Acid Enriched with Thioether Functionality and Versatile Post-synthetic Modifications of Helical β-Peptides

Jungwoo Hong, Wonchul Lee[1], Hee-Seung Lee[*]

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

Herein, we present a novel cyclic β-amino acid featuring a thioether moiety, namely *trans*-(3*S*,4*R*)-4-aminotetrahydrothiophene-3-carboxylic acid (ATTC). This multifaceted β-amino acid serves as a versatile, functional building block for designing β-peptides with well-defined secondary structures. Using a refined synthesis process, we developed various β-peptide hexamers incorporating the ATTC design. Detailed analysis through X-ray crystallography, circular dichroism, and NMR spectroscopy demonstrated that these ATTC-based β-peptides predominantly exhibit 12-helical conformations akin to their isomeric counterparts. Additionally, ATTC's structure allows for intricate modifications after synthesis, with our targeted conjugation methods underscoring its special capabilities. This advancement expands potential applications across diverse research domains. Overall, our study accentuates the pivotal role of ATTC in shaping the cyclic β-amino acid landscape and provides novel insights into synthetic peptides and their broader scientific implications.Reference) *Angew. Chem. Int. Ed.* 2023, e202305196.



Poster Presentation : **ORGN.P-127**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Chiral Recognition in Short β-Peptide Foldamers: Insights from Racemic Mixtures

Seoneun Jeong, Jintaek Gong[1], Hee-Seung Lee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemical Science Education, Sunchon National University, Korea*

Chirality, a fundamental property in nature, plays a critical role in determining the folding and dynamic behavior of proteins and various biomolecules. Predominantly, L-enantiomers of amino acids—essential building blocks of proteins—showcase this inherent chirality in biological systems. Despite over a century of research into chiral recognition, its comprehensive understanding remains a challenge due to the involved complexities.Our study simplifies this exploration by using short β-peptide foldamers with pre-structured helical patterns, sidestepping the complications arising from longer and more intricate peptide sequences. By integrating pyridine units at both ends of foldamers derived from either *trans*-(*S*,*S*)- or (*R*,*R*)-2-aminocyclopentanecarboxylic acid (ACPC) enantiomers, we synthesized unique ligands. When combined in a 1:1 racemic blend, crystallization facilitates the creation of a metal coordination bond between the ligand's end functions and silver ions. Our primary aim is to discern how metal coordination affects the stereoperception of chiral entities. X-ray diffraction outcomes highlight heterochiral and homochiral coordination tendencies, influenced by the chiral ligand's length and specific crystal growth conditions. Investigating racemic mixtures of these varied chiral molecules promises to offer invaluable insights, potentially shedding light on life's origins in future studies.

Poster Presentation : **ORGN.P-128**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Catalytic Asymmetric 1,2-Addition of Borylalkene-Derived Nucleophiles to Imines for Chiral β-Aminoboronate Synthesis

He Jing, Cham Bi Seo[1], Jaesook Yun[1,*]

Chemistry, Sungkyunkwan University, Korea

[1] Department of Chemistry, Sungkyunkwan University, Korea

We report the catalytic asymmetric 1,2-addition of chiral borylalkyl-copper species generated in situ from vinyl boronate containing methylated acenaphthoquinone (mac), a hindered boron ligand, with N-phosphinoyl imines to synthesis β-Aminoboronates. In the presence of a chiral bisphosphine-ligated CuH catalyst, stereoselective addition of chiral boron-α-alkyl intermediate produced stable and isolable β-aminoboronate ester compounds containing two contiguous stereogenic centers in good yield with high diastereo- and enantioselectivity (up to 99:1 dr and 98:2 er). The resulting β-aminoboronate ester was used in various transformations.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-129**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Divergent access to functionalized sulfones or skipped dienes via base-controlled boroallylation of alkenyl sulfones

Minsoo Lim, Dohyun Park, Jaesook Yun[1,*]

department of chemistry, Sungkyunkwan University, Korea

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

Alkenyl sulfone plays multiple roles with finesse to function as nucleophile, electrophile, or radical precursor. In this regard, transition metal-catalyzed functionalization of such compounds has attracted considerable attention in organic synthesis but remains underexplored due to their limited compatibility with transition metals. We investigated a copper-catalyzed borofunctionalization of α, β-unsaturated sulfones, through Michael type addition of Cu-B(pin) catalyst to alkenyl sulfone followed by electrophilic trapping of allyl electrophile to access β-boryl-α-allyl sulfones. This copper-catalyzed tandem reaction proceeds in a highly diastereoselective fashion to give a single diastereomer of the boroallylated product. Furthermore, mechanistic studies revealed that use of a stronger base led to formation of (E)-skipped dienes derived from the boroallylation product.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-130**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Benzoyl Chloride-Catalyzed Reaction of *N*-Acyl Iminophosphoranes: New Synthetic Methodology for Organic Nitriles

Yeongmi Park, Jinhwan Park, Minsuk Kim, Jongwoo Son[1,*]

Department of Chemical Engineering (BK21 FOUR Graduate Program), Dong-A University, Korea

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

Nitriles are important functional group in organic synthesis because these can be utilized as synthetically valuable precursors in the preparation of bioactive small molecules, natural products, and agrochemicals. Conventional synthetic protocols for organic nitriles still have been mostly performed by using toxic reagents such as cyanides and expensive transition metals. Herein, we present a sustainable synthetic method for organic nitriles from *N*-acyl iminophosphoranes using catalytic amount of benzoyl chloride. Moreover, a single-flask synthesis of organic nitriles from dioxazolones exhibited improved sustainability and efficiency compared to traditional multistep protocols.

Poster Presentation : **ORGN.P-131**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Triphenylcarbenium Tetrakis(pentafluorophenyl)borate Enabled Sustainable and Extremely Active Cyanosilylation of Ketones

Muhammad Israr, Han yong Bae[1,*]

Department of Chemistry, Sungkyunkwan University, Pakistan

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

In this presentation, we present the cyanosilylation of ketones using tritylium tetrakis(pentafluorophenyl)borate ([Ph3C]+[B(C6F5)4]–) as an extremely active organocatalyst. The neutral, air- and moisture-tolerant nature of the solid salt is beneficial for user-friendly handling. With this transition metal-free catalytic system, the corresponding cyanohydrin trimethylsilyl ethers could be obtained in quantitative yields with 50 ppm catalyst loading by employing a wide range of ketones as starting materials. Under solvent-free conditions with no temperature influence (cooling or heating) and column chromatography, the gram-scale reaction works excellently, and highly pure products were obtained by removing only the volatiles. Experimental and analytical studies shows that in situ generated silylium with weakly coordinating anion ion-pair as an active catalyst plays a vital role in excellent reactivity.[1]

Triphenylcarbenium Tetrakis(pentafluorophenyl)borate Enabled Sustainable and Extremely Active Cyanosilylation of Ketones

Muhammad Israr, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Republic of Korea. * E-mail: hybae@skku.edu

In this presentation, we present the cyanosilylation of ketones using tritylium tetrakis(pentafluorophenyl)borate ($[Ph_3C]^+[B(C_6F_5)_4]^-$) as an extremely active organocatalyst. The neutral, air- and moisture-tolerant nature of the solid salt is beneficial for user-friendly handling. With this transition metal-free catalytic system, the corresponding cyanohydrin trimethylsilyl ethers could be obtained in quantitative yields with 50 ppm catalyst loading by employing a wide range of ketones as starting materials. Under solvent-free conditions with no temperature influence (cooling or heating) and column chromatography, the gram-scale reaction works excellently, and highly pure products were obtained by removing only the volatiles. Experimental and analytical studies shows that in situ generated silylium with weakly coordinating anion ion-pair as an active catalyst plays a vital role in excellent reactivity.[1]

References

[1] Israr, M.; Bae, H. Y. Green Chemistry, **2023**, *25*, 2387.

Poster Presentation : **ORGN.P-132**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Manganese(I)-Catalyzed *ortho*-selective C-H Alkenylation of Purines Using Terminal Alkynes

Jihye An, Hyeonwoong Bae, Jongwoo Son[1,*]

Department of Chemical Engineering (BK21 FOUR Graduate Program), Dong-A University, Korea

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

6-Arylpurine analogues have demonstrated potential pharmacological activities such as cytostatic, anti-HCV, and antibacterial activities. Previous studies on functionalization of 6-arylpurines has considerably explored using precious transition metals such as palladium, rhodium, and ruthenium. In this poster presentation, we introduce manganese(I)-catalyzed *ortho*-selective alkenylation of 6-arylpurines using terminal alkynes. Alkynes containing aryl, aliphatic, heteroaromatic, and BODIPY motifs apply to the reaction to afford variously alkenylated purines in moderate to excellent yields.

Poster Presentation : **ORGN.P-133**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Solution-Based Synthesis for Large-Scale Peptide Nucleic Acid

Jin woo Jung, In seok Hong[1,*], Minji Kim[2]

Material Dept., Seasunbiomaterials, Korea
[1] *Department of Chemistry, Kongju National University, Korea*
[2] *Kongju National University, Korea*

Peptide nucleic acids (PNAs) are a class of synthetic nucleic acid analogs that have gained significant attention in the field of molecular biology due to their unique properties. PNAs have several features that make them attractive as research tools, including high binding affinity to complementary DNA and RNA sequences, resistance to enzymatic degradation, and a structure that is amenable to chemical modification. However, challenges such as synthesis complexities and low solubility have constrained PNA research. To address these limitations, we have developed a solution-based method for the large-scale synthesis of various modified PNAs aimed at enhancing solubility and more. This innovative approach demonstrates significantly improved yields and purity when compared to conventional methods, effectively overcoming these challenges and paving the way for new directions in PNA research.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-134**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Janus-Type ESIPT Chromophores with Distinctive Intramolecular Hydrogen-bonding Selectivity

Bokyeong Hwang, Juyoung Yoon[1,*], Myung Hwa Kim[*], Sungnam Park[2,*]

Department of Chemistry & Nanoscience, Ewha Womans University, Korea
[1]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*
[2]*Department of Chemistry, Korea University, Korea*

In this study, we introduce a novel family of Janus-type ESIPT (Excited-State Intramolecular Proton Transfer) chromophores characterized by distinct hydrogen bonding preferences within a single molecule. These chromophores exhibit selective interactions with multiple hydrogen bond acceptors (HBAs), with the central hydroxyl group favoring intramolecular H-bonds with imines in imine-modified 2-hydroxyphenyl benzothiazole (HBT) chromophores, while tethering the benzothiazole moiety in hydrazone-modified HBT chromophores. Imine-derived HBTs demonstrate enhanced fluorescence efficiency, whereas hydrazone-derived chromophores display reduced spectral overlap between absorption and fluorescence bands. Quantum chemical calculations elucidate the molecular origins of these biased intramolecular H-bonds and their influence on the ESIPT process. This Janus-type ESIPT chromophore architecture opens up exciting prospects for the design of solid luminescent materials.

Poster Presentation : **ORGN.P-135**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Electron donor-acceptor type delayed fluorescence emitters with inverted singlet and triplet excited states

Jiyun Kim, Youngnam Lee, Soohyeon Lee[1], Eunji Sim[2], Jong-in Hong[3,*]

Seoul National University, Korea

[1]*Yonsei University, Korea*

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

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

Emitters having a negative energy difference between their lowest singlet and triplet excited states are promising candidates for developing next-generation organic light-emitting diodes (OLEDs) because their inverted singlet and triplet (IST) excited states enable exothermic reverse intersystem crossing, which results in a fast rate constant for reverse intersystem crossing and facilitates the efficient harvesting of triplet excitons. This study reports the development of organic emitters comprising 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene as an electron acceptor and 10H-spiro[acridine-9,9'-fluorene] as an electron donor that exhibit IST-excited states. We confirmed the presence of IST excited states in our emitters using photoluminescence spectroscopy, time-correlated single-photon counting, and excited-state density functional theory calculations. In addition, by varying the number of electron donors and the dihedral angles between the electron donor and acceptor, we identified the underlying reasons for the inversion of the singlet and triplet states. Furthermore, we achieved high external quantum efficiencies of up to 30% by utilizing the IST emitters as emitting layers in OLEDs.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-136**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

A Strategy for Enzyme-Responsive Foldecture Construction

Minsang Kang, Hee-Seung Lee*

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

Foldectures, micro-sized 3D structures constructed from noncovalent interactions of peptidic foldamers, present an innovative method to emulate protein tertiary and quaternary structures. Taking advantage of its versatile characteristics, we have demonstrated a *C*3-symmetrical foldecture's potential as a supramolecular delivery system analogous to bacterial microcompartments (BMC)[1]. In this pursuit, we aimed to broaden foldecture's functionality without compromising its delivery capabilities. To this end, we substituted the C-terminal residue of a recognized α/β peptidic foldamer with phosphoserine—hydrolyzable by alkaline phosphatase (ALP) in biological environments. We hypothesized this would initiate an enzyme-instructed morphological transformation (EIMT) of the foldecture. Although we crafted a nanosized sphere-shaped foldecture with this modification, the expected transformation under ALP's influence was absent. Notably, high-resolution mass spectrometry (HRMS) highlighted the hydrolysis of the modified foldamer, distinguishing it from its nonhydrolyzable counterpart. This surprising result underscores foldecture's promise as an enzyme-responsive entity. Upcoming research will dissect this enzyme interaction and probe into the design of stimuli-responsive foldectures.

Poster Presentation : **ORGN.P-137**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Self-Assembly Induced Photosensitization of Long-Tailed Heavy-Atom-Free BODIPY Derivatives for Photodynamic Therapy

Yeju Lee, Juyoung Yoon[1,*]

Chemistry & Nanoscience, Ewha Womans University, Korea

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

Type I photosensitizers (PSs) hold great promise for advancing photodynamic therapy (PDT) due to their ability to generate radicals that remain effective even in low oxygen conditions. Developing highly efficient type I PSs is crucial, and one approach to achieve this is through self-assembly. In this study, a straightforward and efficient method was devised to create heavy-atom-free PSs for PDT using self-assembled long-tailed boron dipyrromethene dyes (BODIPYs). These resulting aggregates, named BY-I16 and BY-I18, effectively convert their excited energy into the triplet state, generating reactive oxygen species that play a critical role in PDT. Moreover, the aggregation process and PDT performance can be controlled by adjusting the length of the alkyl chains in the tails. This concept was demonstrated by showcasing the effectiveness of these heavy-atom-free PSs both in lab settings (in vitro) and in living organisms (in vivo), under both normal oxygen levels and low-oxygen (hypoxic) conditions.

Poster Presentation : **ORGN.P-138**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Temperature controlled divergent synthesis of 2H-pyrrole and oxathiazonine

Juhyun Kim[*], Joungun Park

Department of Chemistry, Gyeongsang National University, Korea

Divergent synthesis is an ideal synthetic strategy for synthesizing other heterocyclic compounds from same starting materials. This synthetic strategy has attracted a great deal of interest because it can improve the efficiency of chemosynthesis. Heterocyclic frameworks are key structural cores in diverse natural products comprised of bioactive and pharmacologically significant compounds. Particularly medium-size ring(8−11-membered ring structures) compounds exhibit a broad spectrum of bioactivity and are widely used in the pharmaceutical industry. However, medium-size ring is difficult to synthesize due to low conformational stability, transannular interactions, bond and torsional strains. In this study, dihydropyrrole synthesized by the palladium catalyzed cycloaddition was used as the starting material. We have developed a strategy for temperature-controlled divergent synthesis using base, allowing for the selective synthesis of five-membered ring compound 2H-pyrrole and nine-membered ring compound oxathiazonine. Furthermore, 2H-pyrrole and oxathiazonine were developed as a tandem reaction without any purification process.

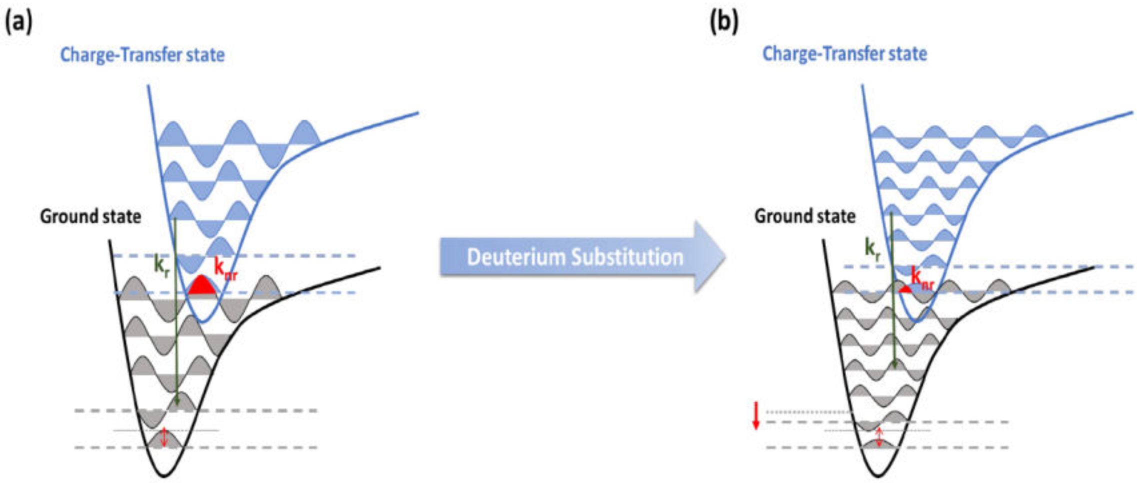
Poster Presentation : **ORGN.P-139**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

STRATEGY FOR REDUCING NON-RADIATIVE RECOMBINATION IN DYE-SENSITIZED SOLAR CELL

Seungrok Kim, Tae-Hyuk Kwon[1,*]

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

Dye-sensitized Solar Cell (DSSC) is one of the attractive solar cells due to its eco-friendly and transparent properties. However, commercialization of DSSCs is limited because of its limited power conversion efficiency (PCE) compared to other solar cells. Several researchers developed strategies to increase the short-circuit current density (Jsc) and open-circuit voltage (Voc). However, the strategy to increase Voc is scarcely investigated. Since the Voc is mainly affected by recombination, caused by radiative and non-radiative relaxation process, these two processes should be suppressed to enhance Voc. Previous research has focused on reducing the radiative recombination, and research to reduce the non-radiative recombination are less investigated. Herein, this research proposes a strategy for decreasing the non-radiative recombination by deuterium substitution for the photosensitizer. The non-radiative recombination is known to be caused by overlapping between the lowest vibrational energy state of the excited state and high-order vibrational energy state of the ground state [1]. The deuterium substitution can decrease the vibrational energy state due to presence of heavy atoms and hence, we anticipate that the deuterium substitution can effectively decrease the non-radiative recombination by decreasing the overlap of the two vibrational energy states (Figure 1). We expect this work contribute to molecular strategy understanding isotope effect on recombination process.


(a)
Charge-Transfer state
Ground state
k_r
k_{nr}
Deuterium Substitution
(b)
Charge-Transfer state
Ground state
k_r
k_{nr}

Poster Presentation : **ORGN.P-140**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Alkyl SuFEx Hubs of Quaternary Carbon Stereogenic Centers via Super Brønsted Base Organocatalysis

Soyeon Kim, Jin Hyun Park[1], Han yong Bae[1,*]

Chemistry, Sungkyunkwan University, Korea

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

The compound sulfonyl fluoride has recently gained attention as a powerful building block in sulfur(VI) fluoride exchange (SuFEx) click chemistry. The challenge lies in creating complex structures involving highly functionalized aliphatic sulfonyl fluorides, which serve as pivotal hubs for SuFEx click reactions through the catalytic formation of carbon-carbon bonds (Csp3-Csp3). We present a successful method for efficiently performing a Michael addition reaction between arylcyanoacetic acid alkyl ester and ethenesulfonyl fluoride (ESF). This methodology is facilitated by the use of super Brønsted base catalysis. The developed protocol exhibits remarkable reactivity when employing superbases such as 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) and related catalysts. This approach can be widely applied to synthesize a diverse range of α-(hetero)arylated cyanoacetates, incorporating carbon-quaternary stereocenters that are crucial in SuFEx hub formation. The method demonstrates its efficiency even under "on-water" conditions, making it adaptable to aqueous environments. The combination of super Brønsted base catalysis and ESF as a reactant has proven to be valuable in accessing intricate molecular architectures through Michael addition reactions. This advancement contributes to the growing toolbox of SuFEx click chemistry, facilitating the creation of novel and complex compounds with potential applications in various fields of science.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-141**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

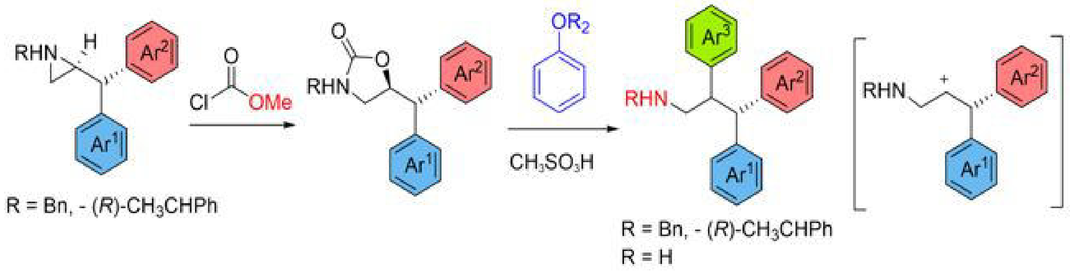
Stereoselective bis-arylation and oxazolidinone-mediated stereoselective tris-arylation from aziridine-2-carboxylate

Seyeon Yoo, Hyun-Joon Ha[1,*]

department of chemistry, Hankuk University of Foreign Studies, Korea

[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Amines bearing diverse aryl substituents as their single monomeric or polymeric forms with potential utility as energy and new materials have been synthesized in a simple and efficient manner from aziridine-2-carboxaldehyde and diverse phenyl groups. Two aryl groups were added via aziridine-2-yl carbanion which was then converted to oxazolidine-2-one as a synthetic intermediate. Then they were further reacted with another aryl group in the presence of BF3OEt2 to yield 3,3,2-triarylpropylamine with the possible benzylic carbanion intermediate.



Poster Presentation : **ORGN.P-142**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Cu-Catalyzed Regio- and Stereoselective Disilylation of 1-Aryl-substituted buta-2,3-dien-1-ols

Hwiwoong Lee, Telma Kamranifard, Soyun Oh, Byunghyuck Jung[1,*], Yunmi Lee[*]

Department of Chemistry, Kwangwoon University, Korea
[1]*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Allylsilanes are valuable intermediates in organic synthesis, serving as versatile allylating agents. They exhibit a remarkable capacity to engage in a diverse array of chemical reactions, thereby enabling the construction of complex molecules. Allyl disilanes are particularly appealing due to their ability to achieve double allylation and enable the modification of two carbon-silicon bonds. In contrast to their synthetic utility, synthetic methodologies involving silylmethyl allylsilanes have received relatively less attention and investigation.In this study, we have devised a double addition of silyl group to 1-(hetero)aryl-substituted buta-2,3-dien-1-ols using silylborane reagents promoted by copper catalyst. This methodology enables the efficient and selective synthesis of a diverse range of α-silylmethyl-(E)-allylsilanes with high regio- and stereoselectivity.

Poster Presentation : **ORGN.P-143**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Copper-catalyzed silylation of allenols with silylborane reagents

Telma Kamranifard, Yeonjoo Lee[1], Yurim Lee[1], Hwiwoong Lee, Byunghyuck Jung[1,*], Yunmi Lee[*]

Department of Chemistry, Kwangwoon University, Korea

[1]*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Organosilicon compounds are of great importance as organic materials with broad applicability both as synthetic intermediates and promising functional molecules within the realm of pharmaceuticals and materials science. Among these, silyl-substituted dienes stand out as versatile foundational building blocks in the field of synthetic chemistry. Silicone-incorporating derivatives find diverse application in numerous chemical processes, encompassing cross-coupling reactions, Diels-Alder reactions, allylation processes, polymerizations, and beyond.Previous methodologies have reported the utilization of silyl zinc reagent and disilane reagent as sources to supply silicon in the silylation of allenol. In this presentation, we introduce a new approach for synthesizing 2-silyl-1,3-butadienes through Cu-catalyzed silylation of readily available allenols using silylborane reagents under mild reaction conditions. Notably, our method accommodates both secondary and tertiary allenols as suitable coupling counterparts. The catalyst system devised in this study shows remarkable efficacy in promoting the production of various functionalized silyl-containing compounds and achieves remarkably high yields while maintaining excellent regioselectivity ratios (>98:2).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-144**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Copper Catalyzed One-Pot Arylation and Cyclization of Diaryliodonium Salts Derived from o-Iodoanilines for heterocycles syntheses.

Miseon Choi, **Chung Whan Lee***

Department of Chemistry, Gachon University, Korea

Diaryliodonium salts have been extensively employed as a versatile and environment-friendly arylating reagent for the syntheses of various heterocycles by its advantageous natures of high reactivity, stability, less toxicity, and easy preparatory procedure.Despite the versatility of diaryliodonium salts, diaryliodonium salts derived from o-iodoanilines have not been widely used to synthesize heterocycles. Diaryliodonium salts derived from o-iodoanilines have bifunctional reactivities of addition and cyclization. So we wanted to make heterocycles easily and simply using this property, and to confirm this, we synthesized indolo[2,3-b]indoles in one-pot.Through this result, we found that the diaryliodonium salt derived from o-iodoaniline can be effectively used for heterocycle synthesis. Accordingly, we are conducting research on the syntheses of other heterocycles.

Poster Presentation : **ORGN.P-145**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Unveiling Metal-Peptide Interactions: Synthesis and Characterization of Histidine-Integrated Foldamer Ligands

Sungmo Koo, Hee-Seung Lee[1,*], Jaewook Kim[1]

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

Proteins in natural systems exhibit a wide range of functions stemming from distinct structural units. There has been significant research into mimicking the structure and function of proteins by manipulating amino acid sequences and secondary structures. Notably, 2-aminocyclopentanecarboxylic acid (ACPC) and 2-aminoisobutyric acid (Aib) stand out for their ability to induce helical structures in short peptide foldamers. Building on this knowledge, we previously utilized foldamer ligands made of ACPC, Aib, and L-methionine, which showed an aptitude for coordinating with CuI clusters. This coordination led to the formation of network structures that featured chiral channels through metal binding, showcasing functionalities rooted in host-guest interactions.ref Our current study advanced this work by synthesizing a series of foldamer ligands that incorporate L-histidine, a known metal-coordinating site. We explored metal coordination capabilities with these newly designed ligands and assessed the affinity between the ligands and metals using UV-Vis spectroscopy. Single-crystal X-ray diffraction (SC-XRD) and circular dichroism (CD) spectroscopy were employed to further elucidate the structure of the ligand-metal complexes. Given our findings, we are optimistic that this new series of foldamer ligands containing L-histidine will lead to identifying innovative, stable metal-peptide network structures via interactions with various metals. These potential discoveries could revolutionize the development of materials, offering unprecedented functionalities and structural features.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-146**

Organic Chemistry

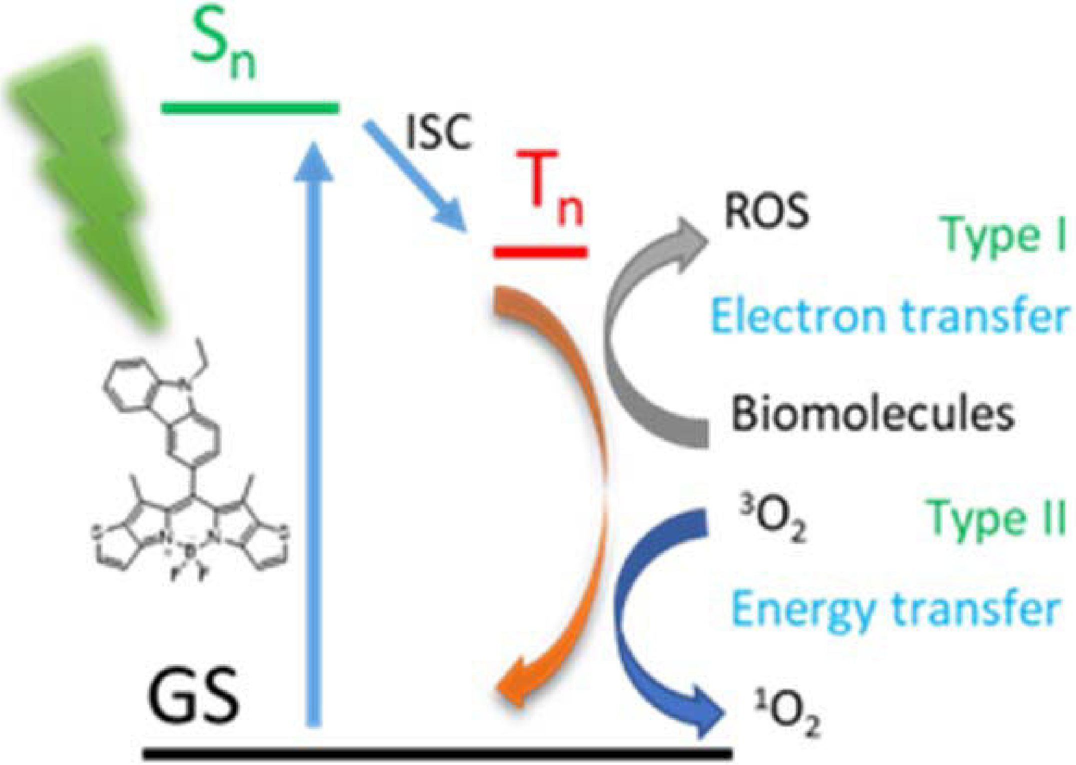
Exhibition Hall C FRI 11:00~13:00

Mitochondria-targeted heavy-atom-free photosensitizers based on thiophene-fused BODIPY for aggregation-induced fluorescence theranostic

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*

Conventional photosensitizers (PSs) used in photodynamic therapy (PDT) have shown preliminary success; however, they are often associated with several undesirable drawbacks. These limitations include the potential dark toxicity in healthy tissues, low efficacy under hypoxic conditions, restricted fluorescence imaging capabilities, and nonspecific targeting during treatment. Consequently, we devised a novel approach to address these concerns by designing a mitochondria-targeted heavy-atom-free PS (Cz-SB) based on thiophene-fused boron dipyrromethene (BODIPY). This innovative PS demonstrates potent generation of reactive oxygen species (ROS) under hypoxia conditions, rendering it highly efficient for hypoxic cancer PDT. Moreover, Cz-SB exhibits excellent biocompatibility and robust fluorescence imaging properties within the mitochondria of living cells, owing to its distinctive aggregation-induced emission characteristics. We believe that the Cz-SB PS holds significant promise as a versatile and comprehensive phototheranostic probe for various cancer types, presenting a potential “one-for-all” solution with future research and clinical studies.We synthesized a heavy-atom-free PS, Cz-SB, by incorporating an electron-rich carbazole group at the meso position of thiophene-fused BODIPY. When exposed to light, Cz-SB exhibited the ability to generate ROS through both type II and type I mechanisms, which are dependent and independent of the oxygen concentration, respectively. In cellular studies, Cz-SB demonstrated excellent biocompatibility, targeted fluorescence imaging in mitochondria, and effective PDT action under hypoxic conditions. These promising results support the potential of Cz-SB as a valuable agent in cancer phototheranostics.


S_n
ISC
T_n
ROS
Type I
Electron transfer
Biomolecules
$^3O_2$
Type II
Energy transfer
$^1O_2$
GS

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

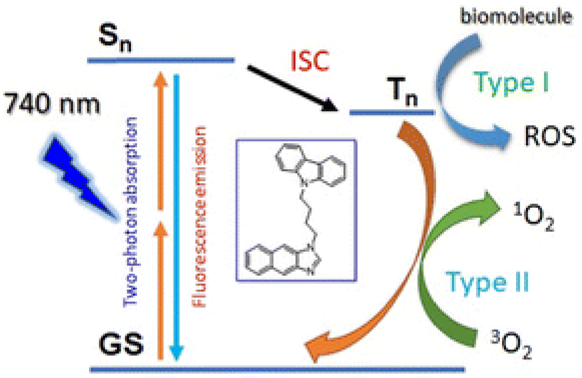
Poster Presentation : **ORGN.P-147**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

A Heavy-Atom-Free Photosensitizer: The Imidazole-Carbazole Conjugate for Two-Photon-Excited Photodynamic Therapy and Fluorescence Imaging

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*

To enhance the process of intersystem crossing (ISC) and the generation of ROS, heavy atoms have traditionally been introduced into PSs. However, concerns regarding the cost and dark toxicity associated with heavy metals have persisted. As a solution, there has been growing interest in the design of molecular structures using heavy-atom-free PSs. Moreover, for PDT treatments to be effective, the absorption wavelength of PSs must fall within the phototherapeutic window (700–900 nm), allowing for adequate tissue penetration of light. However, longer wavelengths (>900 nm) are less efficient in inducing the necessary energy transfer between the triplet excited states of PSs and oxygen molecules. Two-photon excitation offers an alternative approach, enabling PDT based on UV-Vis PSs to extend into the phototherapeutic window, provided that the PSs exhibit a two-photon absorption cross-section ($\sigma 2$) in the near-infrared (NIR) range. Design strategies for enhancing two-photon absorption often involve the expansion of π-conjugation or the introduction of donor and acceptor groups to heavy-atom-free PSs. Nonetheless, challenges such as hydrophobicity and low singlet-to-triplet ISC efficiency remain, limiting their suitability for biological applications.Addressing these complexities, we present a heavy-atom-free photosensitizer termed CI, which is built on the foundation of an imidazole-carbazole conjugate. This CI photosensitizer demonstrates robust fluorescence emission and ROS generation through both type I and II mechanisms. Notably, CI showcases exceptional efficacy in photodynamic therapy and fluorescence bioimaging under two-photon excitation (740 nm), as validated in experiments involving HeLa cells, all while exhibiting negligible dark toxicity.


S$_n$
740 nm
Two-photon absorption
Fluorescence emission
ISC
T$_n$
biomolecule
Type I
ROS
$^1O_2$
Type II
$^3O_2$
GS
N
N
N

Poster Presentation : **ORGN.P-148**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Degradation of Cyano-arenes based Organic Photocatalysts in the presence of amines.

<u>Hyunji Min</u>, Suk Hyun Shin, Miseon Choi, Chung Whan Lee[*]

Department of Chemistry, Gachon University, Korea

Organic photocatalysts offer high structural diversity and eliminate the need for metal removal, addressing the concerns about the toxicity and sustainability of precious metals. Notably, donor-acceptor cyanoarenes, originally developed as thermally activated delayed fluorescence emitters, have gained significant attention due to their unique properties as photocatalysts with high efficiency. Interestingly, several reports demonstrated degradation of such photocatalysts during reactions. Amines, which are often utilized as an electron donor for the generation of radical anions of PCs, also afford alkyl groups or hydrogen for the degradation of PCs. In this research, we tested versatile amines with PCs, which allowed us to discover the degradation behavior for PCs, ultimately leading us to develop a more useful catalytic system utilizing cyano-arenes based organic photocatalysts.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-149**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

[Withdrawal] A method for Synthesis of tri-substituted Pyrazole from β,γ-unsaturated-α-ketoester

Da In Jeong

Organic chemistry, Hanyang University, Korea

- Withdrawal -

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-150**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Functionalized Isocoumarin Derivatives via Base-promoted Dimerization of 2-(Cyanomethyl)benzoyl Fluorides

Serin Hong, Hee Nam Lim[1,*], Inji Shin[*]

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Isocoumarin derivatives exhibit a wide range of biological activities, including antibacterial, cytotoxic, anti-allergic, and plant growth regulatory effects. Isocoumarin moieties are used as important building blocks in pharmaceutical chemistry, appearing in the structures of antibiotics such as Gilvocarcin M, Ravidomysin and Chrysomycin A. Therefore, the development of an efficient synthetic protocol for isocoumarin is of great interest to organic chemists. We investigated base-promoted dimerization of 2-(cyanomethyl)benzoyl fluorides for the synthesis of functionalized isocoumarin derivatives. In the presence of organic amine base, DIPEA, expected isocoumarins were successfully synthesized in good to excellent yields. Furthermore, treatment of the synthesized isocoumarin compounds with NaH provide 6*H*-dibenzo[*c,h*]chromen-6-one derivatives, which are core structures in natural products and biologically active compounds.

Poster Presentation : **ORGN.P-151**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Bifunctional imidazo[1,5-a]pyridine (ImPy)-derived N-heterocyclic carbene (NHC)-palladium catalysts for Buchwald-Hartwig amination

Changmuk Kang, Sukwon Hong*, Junseong Lee[1], Ji Yeon Ryu[2]

Department of Chemistry, Gwangju Institute of Science and Technology, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*
[2]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

Bifunctional imidazo[1,5-a]pyridine(ImPy)-derived N-heterocyclic carbene (NHC)-palladium complexes have been synthesized and characterized. These ImPy ligands are structurally similar to Buchwald biarylphosphine ligands in that they can be equipped with a biaryl moiety, and their sterically demanding environments can be modulated via N-substituents. Moreover, it is easy to introduce additional bifunctionality while maintaining the above properties. The molecular structure of the ImPy-Pd complexes has been identified by single crystal X-ray diffraction study. These novel ImPy-Pd complexes have excellent results for Pd-catalyzed amination reaction. In the presence of sodium tert-butoxide, various aryl, alkyl amines can react with aryl chlorides to form a new carbon-nitrogen bond in high yields within a short time.

Poster Presentation : **ORGN.P-152**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Diarylketones via Palladium-Catalyzed Coupling Reactions between Acylsilanes and Diaryliodonium Salts

Jaehoon Lee, Hyeonbeom Kim, Jaewon Lee, Inji Shin*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Diarylketones are important building blocks in natural products and synthetic intermediates. Although many synthetic efforts have been made to the preparation of functionalized diarylketones, the development of new synthetic methods remains necessary to broaden the scope of the reactions. Transition-metal catalyzed cross-coupling reactions are one of the most efficient method to form new carbon-carbon bonds. We developed a synthetic strategy for the preparation of various diarylketones via carbon-silicon bond activation of acylsilanes in the presence of palladium catalyst. As a coupling partner, diaryliodonium salts, which has higher reactivity as electrophiles in comparison to aryl halides, were employed. After significant optimization, functionalized diarylketones were successfully synthesized in good to excellent yields.

Poster Presentation : **ORGN.P-153**

Organic Chemistry

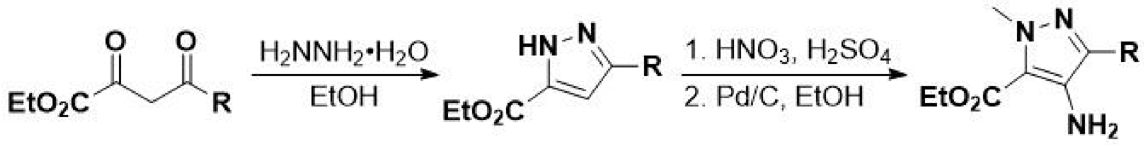
Exhibition Hall C FRI 11:00~13:00

A simple method for synthesis of diversely substituted pyrazole

SeungSu Lee

Department of Chemistry and Center for New Directions in Organic Synthesis, Hanyang University,, Hanyang University, Korea

The pyrazole, a heterocyclic compound, is not known to occur in nature, a variety of its synthesis has been developed. Pyrazoles and its derivatives are widely used in medicine and food industry as dyes and medicinals such as fungicides, insecticides. In this research, a efficient synthesis of diversely substituted pyrazole from simple ketone is described. The advantages of this protocol are simple and high-yielding reaction, step-economy and operationally easy, sustainable approach with the use of readily available starting materials, and high practicality and efficiency



Poster Presentation : **ORGN.P-154**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Correlation between cross-linking density and drug diffusion in thiol-norbornene photopolymerized PEG hydrogels

HyeonBi Jung, Se Won Bae[1,*]

Department of Chemistry and Cosmetics, Jeju National University, Korea
[1]*Department of Chemistry, Jeju National University, Korea*

PEG Hydrogel is a versatile biomaterial that has gained attention in various biomedical applications. It can be formed by cross-linking polyethylene glycol(PEG) with other polymers or molecules. Among these PEG hydrogels, thiol-ene photopolymerized PEG hydrogels have been extensively studied for various biomedical applications such as cell encapsulation, drug delivery and regenerative medicine. Thiol-ene step-growth photopolymerization can be used to tune the hydrogel formation kinetics and network structure by varying the length of the crosslinker. We will provide an overview of the state of the art in thiol-ene photopolymerized PEG hydrogel research and discuss the latest findings on the relationship between crosslinking density and drug release. In addition, we will examine the correlation between various cross-linking densities of PEG hydrogels and the release of two drugs with different isoelectric points. Finally, we will conclude with a discussion of the future direction of PEG hydrogel research and the potential applications of these materials in controlled drug delivery.

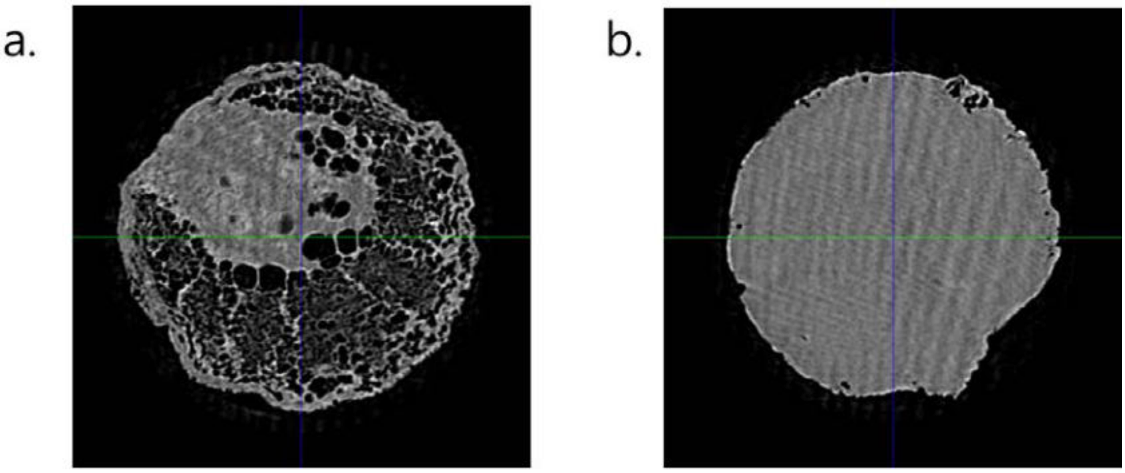


Figure 1. a)Micro-CT image of PEG hydrogel polymerized with 8-Arm 20 kDa PEG-NB and 1.5 eq of HS-10 kDa PEG-SH, b) Micro-CT image of PEG hydrogel polymerized with 8-Arm 20 kDa PEG-NB and 3.0 eq of HS-10 kDa PEG-SH

Poster Presentation : **ORGN.P-155**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Characterization of Cationic Pd Complexes with 2-benzyl-oxazolines as hemilabile coordination

Guldana Issabayeva, On-Yu Kang[1], Seong Jun Park[2], Hwan Jung Lim[2,*]

Medicinal Chemistry and Pharmacology, University of Science & Technology, Kazakhstan
[1]*Korea Research Institute of Chemical Technology, Korea*
[2]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

This poster presents the synthesis and characterization of Pd cationic complexes incorporating mono(2-benzyl oxazoline) ligands. Our research focused on exploring the role of electrostatic interactions of aromatic π electrons of benzyl group for increasing the structural rigidity of cationic Pd complexes. These complexes featured tridentate mono(2-benzyl oxazoline) ligands, where benzyl represents C_6HF_4, C_6F_5, C_6H_5 and C_6H_4Me incorporating a substituted benzyl moiety as a hemilabile coordinating component. Structural examinations of the cationic complexes in the presence of a triflate counteranion revealed that these additional electrostatic interactions have increased structural rigidity, thus enhancing the stability of otherwise labile cationic complexes. This study presents the first example of a cationic Pd complex with 2-benzyl oxazolines highlighting the significance of weak electrostatic interactions in elucidating the three-dimensional structure of a metal complex. This finding holds the potential for the development of catalysts exhibiting improved stability alongside sustained catalytic activity by employing a hemilabile coordination group.

Poster Presentation : **ORGN.P-156**

Organic Chemistry

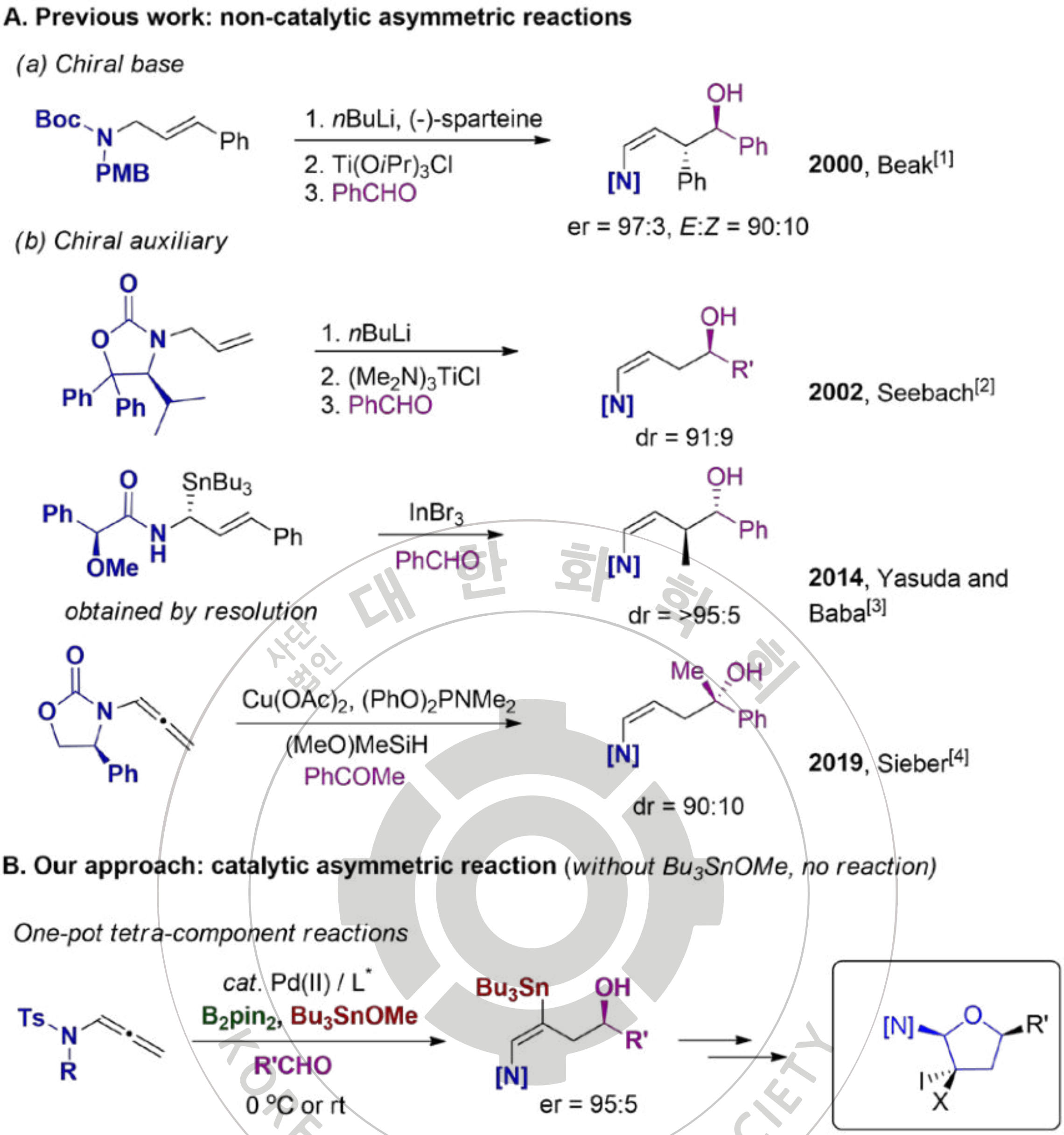
Exhibition Hall C FRI 11:00~13:00

Tetra-component Palladium-catalyzed Asymmetric Diboration of Allenamides: Synthetic Approach to (Z)-δ-Amino Homoallylic Alcohol

Hae Eun Lee, Jin Kyoon Park*, Tae Jun Kim

Department of Chemistry, Pusan National University, Korea

Organo-boron and tin compounds have been considered one of the important building blocks in organic chemistry for decades because of the ability to facilitate C-C bond formation. Recently, these compounds have been introduced to the world though transition-metal catalyzed reaction, particularly asymmetric version. Especially, the Morken group have led the development of palladium-catalyzed asymmetric diboration of allenes, which were expanded by the Ding group to 1,1-disubstituted allenes. Allenamides are a class of molecules containing both allene and amide moieties. The distinctive structural features and reactivity of allenamides make them valuable building blocks for the construction of nitrogen-containing complex compounds. Herein, we report tetra-component palladium-catalyzed asymmetric diboration of allenamides to result in (Z)-δ-amino homoallylic alcohol which could be converted to α-amino tetrahydrofuran with multiple chiral centers. Unusual activation of bis(pinacolato)diboron by tributyltin methoxide to reduce Pd(II) to Pd(0) was studied by phosphorous NMR.KeywordsAsymmetric reaction, diboration, allenamide, tetra-component reaction, chiral amido-ether, 1,4-amino alcohol


A. Previous work: non-catalytic asymmetric reactions
(a) Chiral base
Boc
N
PMB
Ph
1. nBuLi, (-)-sparteine
2. Ti(OiPr)3Cl
3. PhCHO
OH
Ph
[N]
Ph
er = 97:3, E:Z = 90:10
2000, Beak[1]
(b) Chiral auxiliary
O
O
N
Ph
Ph
1. nBuLi
2. (Me2N)3TiCl
3. PhCHO
OH
R'
[N]
dr = 91:9
2002, Seebach[2]
O
SnBu3
Ph
N
H
Ph
OMe
obtained by resolution
InBr3
PhCHO
OH
Ph
[N]
dr = >95:5
2014, Yasuda and Baba[3]
O
O
N
Ph
Cu(OAc)2, (PhO)2PNMe2
(MeO)MeSiH
PhCOMe
Me
OH
Ph
[N]
dr = 90:10
2019, Sieber[4]
B. Our approach: catalytic asymmetric reaction (without Bu3SnOMe, no reaction)
One-pot tetra-component reactions
Ts
N
R
cat. Pd(II) / L*
B2pin2, Bu3SnOMe
R'CHO
0 °C or rt
Bu3Sn
OH
R'
[N]
er = 95:5
[N]
O
R'
I
X

Poster Presentation : **ORGN.P-157**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Exploration of Chiral Phosphine Ligands in Palladium-Catalyzed Asymmetric Silaboration of Allenamide

Tae Jun Kim, **Hae Eun Lee**, **Jin Kyoon Park***

Department of Chemistry, Pusan National University, Korea

Organoboron and organosilicon compounds serve as versatile synthetic building blocks, enabling the synthesis of complicated and sophisticated structures through various reactions such as Suzuki-Miyaura coupling, Hiyama coupling, and Tamao-Fleming oxidation. And allenamide has a more favorable electronic activation than allene and is more stable due to the resonance of the amide group compared to allenamine, which has similar properties but is very unstable. Therefore, we envisioned to install boryl and silyl functional moieties at 1,2-position of allenamide in a single step and succeeded the enantioselective addition of a silicon group to the C1 position using chiral phosphine ligands.During the reaction optimization, we found the best results (86% enantiomeric excess with a 99% yield) with the phosphonite ligands. Our findings revealed that the monodentate ligands are better than bidentate ligands, such as 2,3-O-isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphino)butane (DIOP), and the α,α,α',α'-tetraaryl-2,2-disubstituted 1,3-dioxolane-4,5-dimethanol (TADDOL) structure was found to be suitable as a backbone for the phosphine ligands. Specifically, our exploration mainly based on the phosphoramidite (P-N bond), phosphonite (P-C bond), and phosphite (P-O bond) ligands, all adopting the TADDOL framework. Notably, our investigation revealed the phosphonite ligand as the optimal choice for this transformation. By employing the phosphonite ligand, Pd(dba)2 as the catalyst, and benzotrifluoride as the solvent under mild conditions, we achieved significant efficiency in the asymmetric silaboration of allenamide reaction.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-158**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Photocatalytic hydroxyl radical generation for protein mapping

Chaiheon Lee, Jeong Kyeong Lee[1], Tae-Hyuk Kwon[2,*]

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

Proximity protein labeling, a technique for labeling proteins proximal to a desired spatial point, has been utilized to analyze protein-protein interactions or subcellular localization of proteins. Enzymatic catalysis is broadly used for proximity labeling and subsequent proteome mapping of spatial relationships in cellular organelles. Additionally, a recent study reported that photocatalytic carbene generation to identify protein-protein interaction by using a photocatalyst-antibody system. However, these methods are not appropriate for studying proteome interactions of residual bodies in phagocytosis because these methods depend on enzymes and antibodies. Considering the phagolysosomal environment, it is required to develop chemical tools that label proximal proteins related to residual bodies with high resolution and induce phagocytosis. Herein, we developed photocatalysts that induce phagocytosis and generation of residual bodies. Under temporally controlled light exposure, the photocatalysts could be covalently conjugated to nearby proteins and generate hydroxyl radicals via water-mediated photocatalysis. The produced hydroxyl radicals rapidly labeled nearby proteins, allowing the identification of the protein composition of tertiary lysosome (residual body) of epithelial cells and macrophages. This protein mapping can reveal protein interaction map of residual bodies and interaction with other organelles during phagocytosis.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-159**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

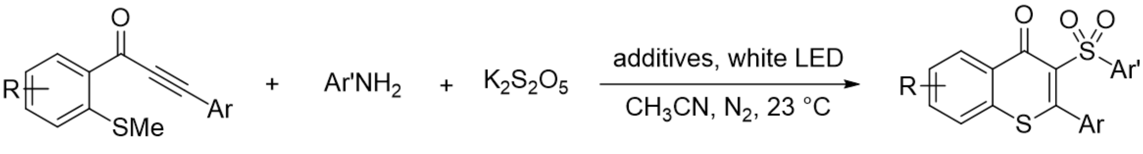
Organophotocatalyzed synthesis of 3-arylsulfonylated thioflavones via in situ activation approach

<u>Sangcheol Na</u>, Anna Lee[1,*]

Department of Carbon Composites Convergence Materials Engineering, Jeonbuk National University, Korea

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

A visible-light-mediated synthesis of 3-arylsulfonylated thioflavones was developed. In this study, potassium metabisulfite was used as a sulfur dioxide surrogate. The desired products were obtained starting from arylamines through an in-situ activation strategy. A visible-light-mediated intramolecular cyclization enables the synthesis of 3-arylsulfonylated thioflavones. This process provides an alternative route for the synthesis of thioflavone derivatives, which have been found in various bioactive compounds.



- ***In-situ generated diazonium salt***
- ***Metal-free***
- ***Three-component reaction***
- ***Visible light, mild conditions***: Reaction temp. 23 °C

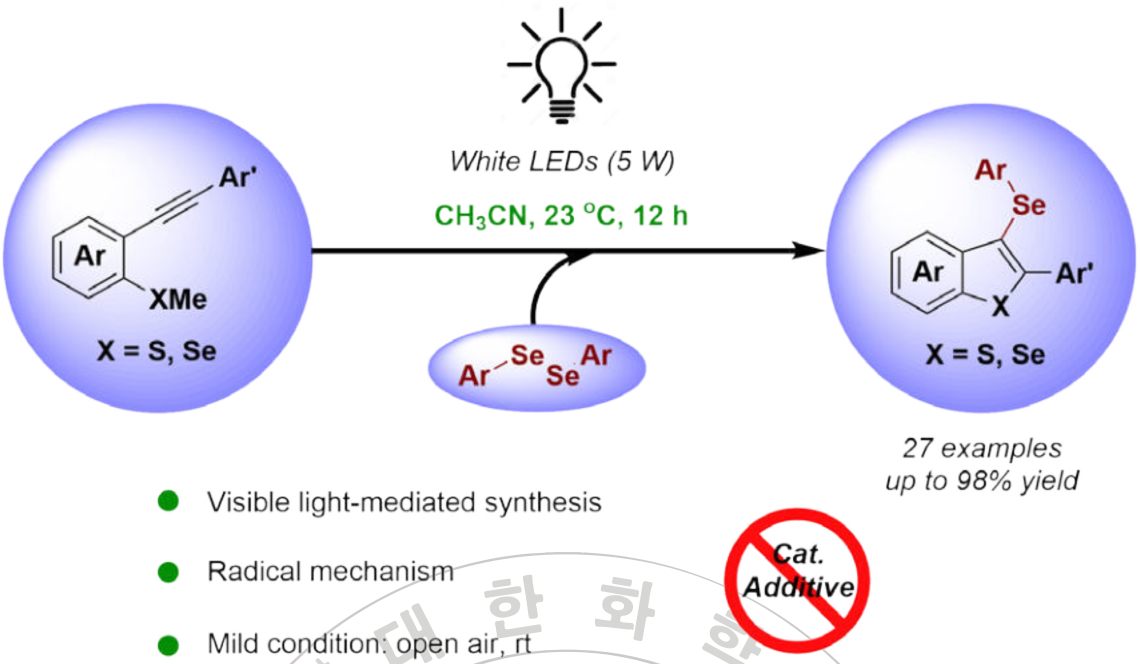
Poster Presentation : **ORGN.P-160**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthesis of 3-Arylselanyl Benzothiophenes via Visible Light-Mediated Radical Cyclization

Sujith Karinkara Periyarath, Anna Lee[1,*]

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

We developed a novel simple and direct method for synthesizing 3-arylselanyl benzothiophenes, which have been found in various bioactive compounds. The reaction proceeded via visible light-mediated radical cyclization. Diaryl selenides were used as aryl selenium sources under the irradiation of white light-emitting diodes (5 W). Moreover, the reactions were conducted under mild conditions, where the desired products were obtained at room temperature (23 ℃) without the need for catalysts or additives. This method allows for an efficient route for synthesizing benzothiophene derivatives, which are crucial scaffolds in organic synthesis.



- Visible light-mediated synthesis
- Radical mechanism
- Mild condition: open air, rt

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-161**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

One-Pot Synthesis of Selenosulfides under Mild Reaction Conditions

<u>Sangik Lee</u>, Anna Lee[1,*]

Department of Carbon Composites Convergence Materials Engineering, Jeonbuk National University, Korea

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

We have developed an efficient one-pot technique for synthesizing selenosulfides, employing organic base catalysts. This strategy facilitates the generation of the desired selenosulfides from readily available starting materials under mild reaction conditions. The need for excess oxidants or additives is eliminated, thereby simplifying the synthesis procedure.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

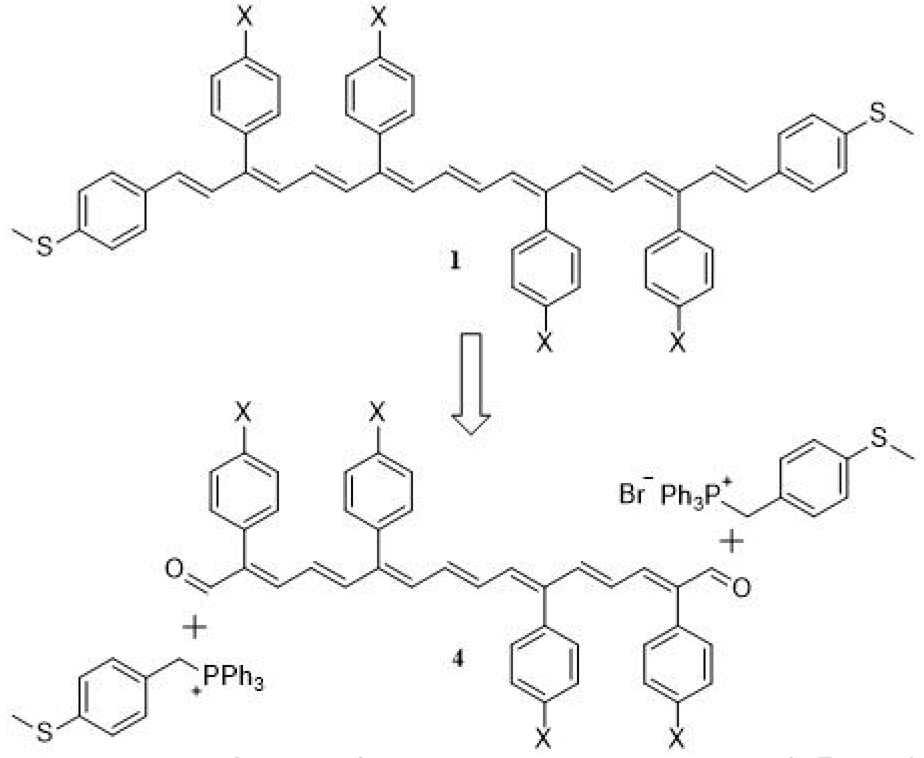
Poster Presentation : **ORGN.P-162**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthetic Strategy for Tetraphenyl-Substituted All-*E*-Carotenoids as Molecular wire

Chibeom Seo, Sangho Koo[*]

Department of Chemistry, Myongji University, Korea

Carotenoids containing phenyl substituents in the polyene chain provide improved stability as well as various electron-conducting abilities to the chain. We synthesized 9,9´,13,13´-tetraphenyl-substituted polyene chains of carotenoids and measured their conductivity. 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.


X
X
S
S
1
X
X
X
X
Br⁻ Ph3P⁺
S
+
O
O
+
PPh3
+
S
4
X
X

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-163**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Grifolin synthesis optimization via C-alkylation of 5-methylcyclohexane-1,3-dione

<u>Han Seunghyo</u>, Sangho Koo[*], Bo-ram Lim[1,*]

Department of Chemistry, Myongji University, Korea

[1]*Bangmok College of General Education, Myungji University, Korea*

Grifolin is a biological active natural product that can be extracted from mushroom, Albatrellus dispansus. It has the effect of suppressing or blocking the cancer cell promoting process.Grifolin is consisted of farnesyl group and orcinol. We tried to synthesize it using Friedel-craft alkylation, but there were problems of regio-chemistry in orcinol and further cyclization in farnesyl group. So, Using the 5-methylcyclohexane-1,3-dione instead of the structure of resorcinol, We solved the regio-chemistry problem, and studied O-alkylation vs C-alkylation of dione and farnesyl chain. Our detail method and result can be found in the poster.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-164**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Apocarotenals of Phenolic Carotenoids for Superior Antioxidant Activities.

Yang Liu, Sangho Koo[1,*]

Department of Chemistry, Myongji University, China

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

We prepared a series of para-phenolic carotenes 1 with ortho- and meta-substitutions and the corresponding apo-12´-carotenals 2. The conjugated aldehyde group in apo-12´-carotenals 2 can improve the conjugation effect of para-phenolic radical with polyene chains. Apo-12´-carotenals 2b and 2c without ortho-substituents exhibited superior antioxidant activities to their corresponding symmetrical carotenes 1 as well as β-carotene and apo-12´-β-carotenal in ABTS and DPPH radical scavenging assays.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-165**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Application of Mn(III)/Co (II) catalyzed oxidation-synthesis of benzofuran and derivatives

Tang Ting, Sangho Koo[1,*]

Department of Chemistry, Myungji University, China
[1]Department of Chemistry, Myongji University, Korea

The benzofuran structure widely exists in biologically active natural products and is the core skeleton for drug development. A large number of studies have shown that benzofuran compounds have strong antitumor, antibacterial, antioxidative, antiviral and other biological activities, making it as potential natural drug lead compounds.A new methodology for the synthesis of benzofuran derivatives has been devised.Furans that incorporate a β-ketoester moiety at the 2-position experience oxidative ring-opening facilitated by Mn(III)/Co(II) catalysts in the presence of an oxygen environment. This reaction leads to the generation of 1,4-dicarbonyl functionalities through the intermediacy of an endoperoxide species. Subsequently, a sequential cyclization by β-ketoester unit provides the formation of 4-hydroxy-2-cyclohexen-1-ones. These oxidation/cyclization products are adeptly converted into versatile benzofuran derivatives via consecutive aromatization and Paal–Knorr reaction sequences.

Poster Presentation : **ORGN.P-166**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Biomass conversion synthesis to pyralline platform through one-pot reaction of ribose and amino acids and synthesis of various pyrrole alkaloid derivatives

Huisu Yeo, Sangho Koo[*], Bo-ram Lim[1,*]

Department of Chemistry, Myongji University, Korea

[1]*Bangmok College of General Education, Myungji University, Korea*

We propose a method for producing Pyrrole-2-carbaldehyde by one-pot conversion of L-amino acid and the reducing sugar D-Ribose. Through this, many derivatives using Pyrrole, which are widely used in medical chemistry, were synthesized. Several types of Pyrrole derivatives have been designed from Pyrrole-2-carbaldehyde. Piperazin-2-one was synthesized through a reduction reaction with Benzylamine and further Cyclization with ethane-1,2-diamine. In addition, a method was proposed of synthesizing new structures of Oxazolidine and Piperazin-2-one by reacting with L-Alaninol, Valninol, and Phenylalaninol. We tested these various substances for their anti-inflammatory effects of MTT and Griess.

Poster Presentation : **ORGN.P-167**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthesis of diglycerides using bioactive organic substances

JiSu Hong, Sangho Koo[1,*]

Department of Chemistry, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Bioactive organic substances have excellent effects on human body's antioxidant, anti-cancer, antibacterial, whitening, and anti-aging effects. Combining these compounds to have various efficacies has been a great effort in synthesizing cosmetics and pharmaceuticals. However, when directly bonded in practice, the functional group is lost and the effect is lost. To improve this, a diglyceride having a hydroxyl group capable of combining the two materials and interacting with the functional group was designed. First, after adding epichlorohydrin, ring opening was effectively performed using a BuNBr catalyst to synthesize 1,3-diglyceride. In addition, 1.2-diglyceride was synthesized using the attachment and detachment of the 1.3-acetalglycerin protecting group.

Poster Presentation : **ORGN.P-168**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Palladium-Catalyzed S-allylation of Allylic Alcohols as a Highly Effective Method for Synthesis of Carotenoids by Julia-Kocienski Olefination

Aleksei Golikov, Sangho Koo*

Department of Chemistry, Myongji University, Korea

A mild and generally high-yielding approach for palladium-catalyzed S-allylation by 2-mercaptobenzathiazole of allylic alcohols is described. The synthetic utility of the resulted benzothiazole sulfides was demonstrated by the synthesis of carotenoids such as β- and ε-carotenes and 9’-Z-phenyl-carotene through Julia-Kocienski olefination with high efficiency. Additionally, the discovered selective transformation of allylic alcohols, rather than allylic acetates, makes possible the preparation of naturally occurring xanthophylls such as lutein, zeaxanthin and isozeaxanthin.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-169**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Practical efficient synthesis of Dichloroglyoxime

<u>Hae-Wook Yoo</u>, SeungHee Kim, So Jung Lee, Kuktae Kwon[*]

Agency for Defense Development, Korea

Dichloroglyoxime(DCG) is a key intermediate for the preparation of Dihydroxylammonium 5,5'-bistetrazole-1,1'-dioxide(TKX-50) and other tetrazole based energetic materials. Historically, DCG has been prepared using chlorine gas or N-chlorosuccinimide (NCS). However, all of these methods involve solvent evaporation, which is costly and unsuitable for scale-up. Here in, we developed a new synthetic procedure for the extraction- and evaporation-free, scale-up-friendly synthesis of DCG. Our method proceeds under high concentrations of NCS and dimethylformamide (DMF), and water is used as the only workup material.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-170**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

The Synthesis of Disubstituted Cyclic Ethers via Pd-Catalyzed Intermolecular Oxidative Cyclization Cascade.

Yong Ho Lee*, Yumin Kim[1]

Department of Chemistry, Korea University, Korea

[1]*Chemistry, Korea University, Korea*

Cyclic ethers, specifically tetrahydrofuran (THF) derivatives are known to be privileged scaffolds in a wide range of natural products, pharmaceuticals, and materials. For these reasons, many studies have been conducted to develop efficient strategies for synthesizing polysubstituted THF scaffolds with a high degree of regio- and stereoselectivity. However, these protocols often restricted to intramolecular reactions using specifically engineered substrates. Herein we present the development of a palladium-catalyzed diastereoselective 2,4-dicarbofunctionalized THFs synthesis via intermolecular oxidative cyclization of alkenes and allyl alcohols.

Poster Presentation : **ORGN.P-171**

Organic Chemistry

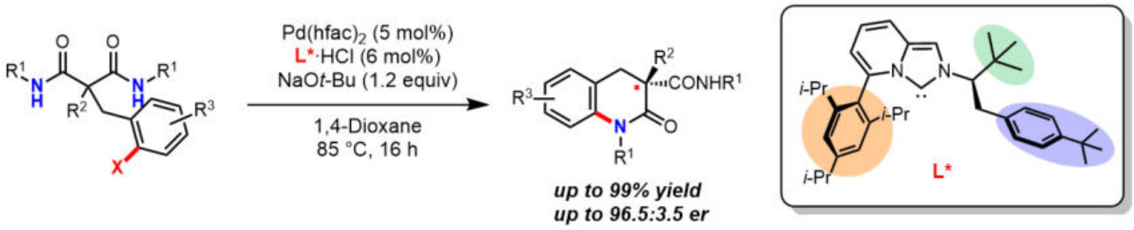
Exhibition Hall C FRI 11:00~13:00

A Bulky Chiral Imidazo[1,5-a]pyridin-3-ylidene Ligand Enabling Pd(II)-Catalyzed Enantioselective Desymmetrization Reaction and Enantioselective Synthesis of 3,4-Dihydro-2-quinolinone to All-Carbon Quaternary Stereocenters.

Woosong Han, Huijeong Ryu, Sukwon Hong*

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

3,4-dihydroquinolin-2-one compounds are an important scaffold found in a core skeleton in natural products and drugs. A palladium-catalyzed enantioselective desymmetrization has been developed with the employment of a bulky chiral imidazo[1,5-a]pyridin-3-ylidene ligand, affording a series of 3,4-dihydroquinolin-2-ones bearing all-carbon quaternary stereocenters in good yields and enantioselectivities. Key to the success of the transformation was the development of a sterically hindered, readily accessible and tunable N-heterocyclic carbene ligand.



Poster Presentation : **ORGN.P-172**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

A novel synthesis of quinazoline derivatives by polymer-supported methodologies

Chang Sang Moon[*], **Jae Yeol Lee**[*]

Department of Chemistry, Kyung Hee University, Korea

A novel method for appending quinazoline to a polymer support via a benzotriazolyl linkage has been developed. The chemistry hinges on the formation of quinazoline. Reaction of in situ formed quinazoline with polymer-supported benzotriazole then results in attachment of the quinazoline to the support. The reactive polymer-supported quinazoline can be subjected to nucleophilic substitution reactions that also cause cleavage of the products from the support.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-173**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

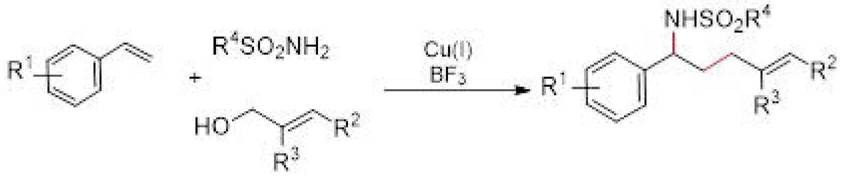
An Eco-Friendly Route to Access 4,5-Unsaturated Sulfonamides via Three-Component Alkene Carbo-Sulfonamidation.

Waqar Ahmed, Pil Seok Chae[1,*]

Department of Bionano Engineering, Hanyang University, Pakistan

[1]*Department of Bionano Engineering, Hanyang University, Korea*

Though sulfonamides hold significance in biological systems, their structural diversity is restricted due to limited availability of synthesis methods.1-5 Recently, the utilization of alkene functionalization has drawn attention as a means to synthesize sulfonamides due to their widespread accessibility and use in organic synthesis. However, the alkene reactions often encounter challenges related to either regioselectivity or the need for substantial reagent quantities. We introduce an innovative and eco-friendly approach to achieve the preparation of 4,5-unsaturated sulfonamides by employing arylalkenes, allylic alcohols, and commercially available sulfonamides. This approach relies on employing a copper (I)-BF3 catalyst pair for alkene functionalization. The catalyst serves a dual purpose: stabilizing the allyl cation and activating the alkene. Diverse allylic alcohols, arylalkenes, and sulfonamides were compatible with the optimized reaction conditions. Furthermore, the resulting products can undergo further structural modifications by utilizing reactive functionalities on allylic alcohols, arylalkenes and sulfonamides.



Poster Presentation : **ORGN.P-174**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

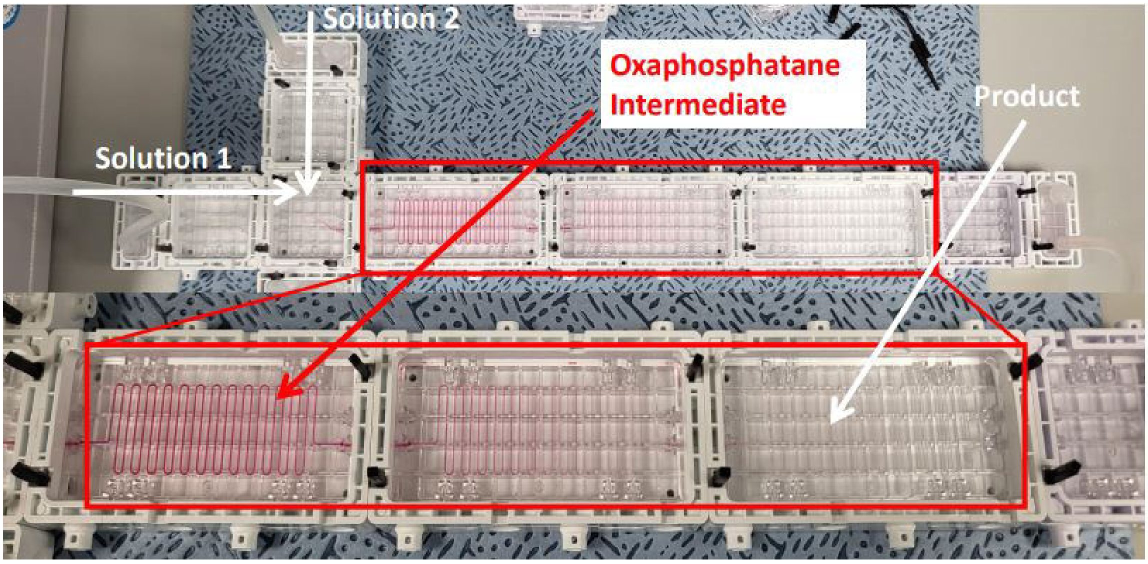
Education Application of Wittig Reaction Using Modular Microfluidic Chip

Chul Soon Park[*], **Young Hwan Jung**[1,*]

Department of Bio-Nanomaterials, Bio Campus of Korea Polytechnics, Korea

[1]*Department of Bio-Nanomaterials, Bio Campus of Korea Polytechnics , Korea*

The flow chemistry has the advantage of being able to process all toxic and corrosive reagents in a closed system, and it is possible to proceed with a highly reproducible organic process by controlling the concentration, temperature, and pressure. In this research results, we designed and prepared a novel modular microfluidic chip reactor for organic synthesis and applied it to the Wittig reaction to confirm successful organic synthesis. Additionally, as the Wittig reaction proceeded, we observed the formation of oxaphosphatane of red color, a four-membered ring intermediate, which is an intermediate produced by the mechanism. The Wittig reaction is also applied to the synthesis of organic and natural substances and is used in the production of various products in the chemical and pharmaceutical industries. Futhermore, We believe that flow chemistry at organic reactions can be used as an educational program for undergraduate students.


Solution 2
Oxaphosphatane
Intermediate
Solution 1
Product

Poster Presentation : **ORGN.P-175**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Fenoprofen-lipoic acid derivatives for butyrylcholinesterase inhibitor

Sung ha Hwang, Da Yeon Song, Min Kyung Shin, Dabin Jeong, Jeong Ho Park[1,*]

Hanbat National University, Korea

[1]*Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea*

Alzheimer's disease is a complex and multifactorial neurodegenerative disorder. The development of drugs for Alzheimer's disease is a complex and challenging process. Alzheimer's disease Pathology involves multiple pathological processes, including the accumulation of beta-amyloid plaques, tau protein abnormalities, neuroinflammation, synaptic dysfunction, and neuronal loss.Drug development strategies for Alzheimer's disease are targeting amyloid Beta, Tau Protein modulation, anti-inflammatory and neuroprotective agents, synaptic dysfunction and neuroprotection, neurotransmitter systems (cholinesterase Inhibitors), mitochondrial function and energy metabolism, etc. Since a single target isn't enough to develop drug candidate, combination therapies involving multiple targets or mechanisms of action are recently noticed for new drug candidates. We have tried to synthesize new type of drug candidate for AD treatment. We reported the synthesis of hybrid compound between fenoprofen (nonsteroidal anti-inflammatory drug) and lipoic acid by using two different linkers, 2-(piperazin-1-yl)ethanol (linker A) and 2-(2-aminoethoxy)ethanol (linker B). Only the hybrid compound using not linker B but linker A showed the inhibitory effect against butyrylcholinesterase (BuChE). From the docking study, we find out that the compound using linker A had the increased bind energy compared to non-salt compound formed using linker B. It may result from forming the ammonium salt inside linker A at the physiological condition.

Poster Presentation : **ORGN.P-176**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Melamine-cored Glucosides (MGs) for Membrane Protein Stabilization

<u>Ehsan Muhammad</u>, Pil Seok Chae[1,*]

Department of Bio-Nano Engineering, Hanyang University, Korea

[1] *Department of Bionano Engineering, Hanyang University, Korea*

Membrane proteins are bio-macromolecules that constitute ～60% of current drug targets. Over the past decade, we have witnessed a number of technological advancements, techniques, and reagents for membrane protein structural biology, resulting in an ever-growing number of membrane proteins with known structures. Before being analyzed by structural, biochemical, and biophysical methods, these bio-macromolecules first need to be extracted from the cellular membranes using amphiphilic molecules called detergents. Detergent-extracted membrane proteins are subjected to structure analysis, but use of classical detergents often leads to loss in the native protein conformations and/or biological activity. As a result, many efforts have devoted to develop new amphipathic agents with enhanced efficacy for membrane protein stabilization. Here, we synthesized a set of glucoside detergents with a melamine core, designated melamine-cored glucosides (MGs). Due to the ability of the melamine core to form hydrogen bonding, these new detergents were capable of forming a dynamic water-mediated hydrogen-bond network between detergent molecules, as supported by molecular dynamics simulations. When evaluated with a set of membrane proteins, MG-C11 conferred notably enhanced stability to the tested proteins including GPCRs compared to commonly-used DDM and LMNG. This result suggests that the water-mediated hydrogen-bond network formed by MG-C11 plays a critical role in enhancing protein stability. Thus, this study not only introduces a novel detergent tool useful for protein structural study, but also provides a new strategy to develop next generation detergents for membrane protein science.

Poster Presentation : **ORGN.P-177**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

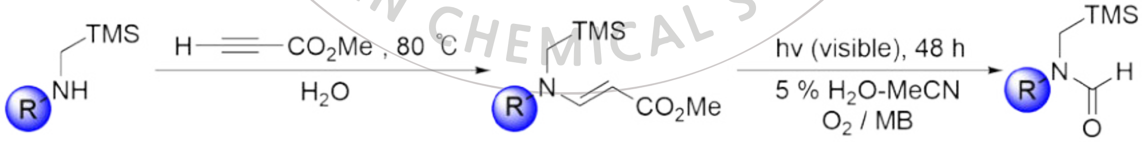
Photosensitized Oxygenation of Oxophilic Silyl Group Containing Electron-Deficient Enaminoester: Direct Access to Aldehyde Formation

Ha Yeon You, Dae won Cho[1,*]

Major of Chemistry, Yeungnam University, Korea

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

Primary amines which have allyl or alkyl group are substituted with Silyl groups. Secondary amines react with Acetylene compound 'Methyl propiolate' under the condition of water by heating and enamine compound is synthesized. Subsequently, When the enamine compound is irradiated with visible light in oxygen conditions through the photocatalyst 'Methylene blue', the alkene chain is cleaved and an aldehyde group is formed.



Poster Presentation : **ORGN.P-178**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Intramolecular Cyclization of *N*-Cyano Sulfoximines by N-CN Bond Activation

Eunsil Kim, Jiyoung Hyun[1], Song Jiho[2], Hwan Jung Lim[*], Seong Jun Park[*]

Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea
[1] *data convergence drug research center, Korea Research Institute of Chemical Technology, Korea*
[2] *medicinal chemistry, University of Science & Technologg, Korea*

The introduction of a sulfoximinoyl moiety into a heterocyclic ring system remains challenging to various disadvantages, such as the requirement for harsh reaction conditions and expensive reagents and catalysts. To this end, we have developed a method for the intramolecular cyclization of *N*-cyano sulfoximines *via* the addition of metal-free halogenated anhydrides to promote the reaction. Our method, which does not require catalysts or expensive reagents and can be performed at room temperature, resulted in excellent yields of the desired thiadiazinone 1-oxides.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-179**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

PET Mechanism-Based Ratiometric Dual-Emissive Fluorescent Probe for the Detection of H2S

Na Yoon Kim, Min Hee Lee[1,*]

Sookmyung Women's University, Korea

[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Hydrogen sulfide (H2S) is a redox molecule and endogenous gas transmitter that, plays a crucial role in various physiological and cellular protective functions in biological systems. Recent literatures revealed elevated expression levels of H2S-producing enzymes in various types of cancers. On the other side, H2S is a nature gas generated from minerals, petroleum industry, and microbial decomposition of organic matters. Due to its harmfulness, the exposure level is strictly regulated. Thus, accurate and precise detection of H2S both in environments and bio-systems is highly demanded.In our research, we developed a ratiometric dual-emissive fluorescent probe for detecting H2S. The probe was constituted in a combination of two fluorophores, nitrobenzofurazan-contained naphthalimide and pyrene. Initially, probe exhibited single emission at 377 nm from the pyrene moiety. However, in the presence of H2S, probe showed two emissions at 530 nm and 377 nm corresponding to the naphthalimide and pyrene moieties, respectively. The detection limit for H2S was calculated to be 0.8 μM. This ratiometric fluorescence response could be explained based on a photoinduced electron transfer (PET) mechanisms. This study is ongoing, and we expect this probe can be applicable to detect H2S in various analytical conditions.

Poster Presentation : **ORGN.P-180**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Conversion from 5-Hydroxymethylfurfural (HMF) to 2,5-Diformylfuran (DFF) through Continuous Flow System

Yea Seul Jang, Chan Pil Park[1,*]

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

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

2,5-Diformylfuran (DFF) is widely known as the most valuable biomass-derived platform, with potential applications including pharmaceutical intermediates, antibacterial agents, organic conductors, etc., and numerous studies are being conducted to produce them. In particular, oxidation of 5-hydroxymethylfurfural (HMF) to DFF is widely known, but there is a disadvantage in that various by-products such as 2,5-furandicarboxylic acid (FDCA) are also produced. Until now, efforts have been made to improve the selectivity of DFF through various studies on solvents, catalysts, and oxidizing agents. Among them, a heterogeneous catalyst such as metal was introduced into the packed-bed method of the continuous flow system to increase the selectivity of DFF. However, there was a problem that humins, a by-product produced, was adsorbed on the surface of the catalyst, and caused inactivation of the catalyst. Therefore, in this study, HMF was converted to DFF without using the heterogeneous catalyst such as metals in the continuous flow system.

Poster Presentation : **ORGN.P-181**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Exploring NO Involvement in Autophagy and Ferroptosis via a Lysosomal-Targeted Fluorescent Probe

<u>Sun Young Park</u>, Min Hee Lee[*]

Department of Chemistry, Sookmyung Women's University, Korea

Organelle-selective bioorthogonal fluorescent chemosensors are indispensable chemical tools for investigating live cell processes involving the sensors' target metabolites. In this study, we developed a lysosomal NO-selective chemosensor (Lyso-NO), composed of a 4-(4-nitrophenyl)thiosemicarbazide-linked naphthalimide and a morpholine moiety as an NO-mediated fluorogenic reporter and a lysosome-targeting unit, respectively. Upon selective reaction with NO in solution and within live cells, Lyso-NO showed a strong fluorescence intensity at 550 nm, and its predominant lysosomal location was revealed by confocal microscopy. Further, lysosomal NO increase was demonstrated to be deeply involved in autolysosome formation during autophagy, and in ferroptosis. Lyso-NO was considered to act as a lysosomal NO-selective sensor, allowing for the bioorthogonal analysis of lysosome-related biological processes.

Poster Presentation : **ORGN.P-182**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Design of a double-locked fluorescent probe for selective imaging of NTR and H_2S in hypoxic cancer cells

Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Hydrogen sulfide (H_2S) is a crucial redox molecule and endogenous gas transmitter, physiological and cellular protective functions in biological systems. Nitroreductases (NTR) are flavoenzymes that catalyze the NAD(P)H-dependent reduction of the nitro group on nitroaromatic compounds and play a key role in the detoxification of carcinogens. Recently, some literatures have reported that the NTR activity and H_2S increase under hypoxia in cancer cells.In this study, we developed a dual-sensitive probe (1) capable of providing a fluorescence response to H_2S and NTR in living cells. Probe 1 is equipped with the naphthalimide as a signal unit and two different recognition moieties, H_2S-sensitive 7-nitro-2,1,3-benzoxadiazole (NBD) and NTR-sensitive 4-nitrobenzyl ester groups. Probe 1 showed emission at 547 nm in the presence of both H_2S and NTR respectively. Moreover, probe 1 showed selective and sensitive detection ability for H_2S and NTR in solution and it was applicable to various cell lines such as breast, prostate, liver, and gastrointestinal origin cancer. In addition, through $CoCl_2$-induced hypoxia and 3D spheroid experiments, it was found that probe 1 could image H_2S and NTR under hypoxia.

Poster Presentation : **ORGN.P-183**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Simultaneous fluorescent detection of hNQO1 and NTR in hypoxic cancer cells using a single probe

Sojin Hong, Min Hee Lee[1,*]

chemistry, Sookmyung Women's University, Korea

[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Human NAD(P)H quinone oxidoreductase (hNQO1) is a flavoprotein that catalyzes the NAD(P)H-dependent reduction of diverse substrates, including quinones. Nitroreductase (NTR) is a flavoenzyme that catalyzes the NAD(P)H-dependent reduction of the nitro group on nitroaromatic compounds and play a key role in the detoxification of carcinogens. Recently, some literatures have reported that the NTR activity and hNQO1 increase under hypoxia in cancer cells.In our research, we developed the dual sensing fluorescent probe 1 for imaging hNQO1 and NTR in hypoxic conditions. The probe 1 was constituted in a combination of fluorophore, TLQ and nitrobenzyl moiety. Probe 1 showed emission at 475 nm and 550 nm in the presence of hNQO1/NADH and NTR/NADH, respectively. This study is ongoing, and we expect probe 1 can be applicable to hNQO1 and NTR-associated disease models.

Poster Presentation : **ORGN.P-184**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Cellular Redox Dynamics Study Using a Dual-Sensing Bioprobe for Hydrogen Sulfide and Hydrogen Peroxide Detection

Songyi Yoo, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Hydrogen sulfide (H_2S) is a gasotransmitter endogenously produced in human body, and it plays crucial roles in cell growth, blood vessel neuromodulation, apoptosis, and anti-inflammation.[1] Hydrogen peroxide (H_2O_2) is a typical ROS produced from the mitochondrial respiratory chain, which participates in various physiological processes such as cell proliferation, differentiation, and hypoxia signal transduction.[2] These two factors are particularly involved in cellular redox balance. For examples, H_2S is overexpressed in ROS-induced oxidative stress conditions. Accordingly, it is important to develop H_2S and H_2O_2 sensitive dual-sensing fluorescent bioprobes to image H_2S and H_2O_2 within cells. Previously, dual-detection probe for H_2S and $H_2O_2$was reported using two sensitive fluorophores, but the fluorescence intensity was interfered with other factors such as FRET phenomenon, making inaccuracy in the H_2S and H_2O_2 detection.[3] In this study, we tried to develop dual-sensing bioprobe for H_2S and H_2O_2 without interfering by FRET, leading to strong fluorescence intensity. Using this system, we aimed to gain insights into the intricate interplay between H_2S and H_2O_2 in cells under various pathological stimuli.References1.Yoo S.; Gopala L.; Kang C.; Lee, M., *Bull. Korean Chem. Soc.*, 2022, *43*, 1231-1235.2.Lee J.; Yoon S.; Chun J.; Kang C.; Lee M., *Anal. Chim. Acta*, 2019, *1080*, 153-1613.Nithya, V.:, Natesan, T.;, Kondapa N.; Arup P.; Shu-Pao W., Sankarprasad B. , *J. Photochem. Photobiol. B.*, 2019, *191*, 99-106.

Poster Presentation : **ORGN.P-185**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Dual-functional Fluorescent Probe to simultaneously detect adenosine triphosphate ATP and hypochlorite ion (ClO–), in living cells and Drug-Induced Liver Injury mice model.

Fortibui Maxine Mambo, **Min Hee Lee**[1,*]

Chemistry, Sookmyung Women's University, Korea

[1] *Department of Chemistry, Sookmyung Women's University, Korea*

Herein, we present a dual functional fluorescent probe RATP-NClO which is capable of detecting adenosine triphosphate (ATP) and hypochlorite ion (ClO–), using two differeent channel. RATP-NClO features a rhodamine unit bearing diethylentramine which can bind to ATP causing an opening of the spiro lactam ring upon excitation at 520 nm resulting to a highly fluorescent product RhA (λex/em = 520 nm /587 nm). On the other hand, the thiomorpholine bearing napthalimide can undergo oxidization in the presence of ClO– when excited at 420 nm to obtain NH (λex/em = 420 nm /534 nm). RATP-NClO further displayed excellent results in monitoring ATP and ClO–, levels in living cells and during drug induced liver injury.

Poster Presentation : **ORGN.P-186**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Pyridoquinolones for Organic Electronic Applications

Hyein Im, Younghun Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Polyheterocyclic molecules are promising candidates for optical and electronic applications when endowed with high photo- and/or electrochemical stability. Quinacridone (QA) is a representative example, which finds utility in organic light-emitting diodes (OLEDs), organic solar cells (OSCs), and organic field-effect transistors (OFETs). Taking the functional core motif of QA, we have developed a new class of polyheterocyclic molecules, pyridoquinolones (PQs). With the extensively π-conjugated structure as a formal fusion of pyridone and quinolone, the nitrogen atoms and carbonyl groups of PQs function as oxidation and reduction sites, respectively, of the bipolar material. Based on this structural design, *trans*-PQ is anticipated to display bipolar redox activity, as both catholyte and anolyte of symmetric redox flow batteries (RFBs). Unlike the trans-isomer, computational studies predicted that *cis*-PQ has a distinct spatial separation of HOMO and LUMO, to produce a small single–triplet energy gap for thermally activated delayed fluorescence (TADF). This presentation will discuss the design principles, synthesis, and electrochemical and photophysical studies of pyridoquinolones as potentially useful materials for symmetric RFBs and TADF emitters.

Poster Presentation : **ORGN.P-187**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Photo-Cleavable Azo Surfactants

Namsoo Lee, Yujin Jo[1], Byeong-Seon Kim[1,*]

School of Education, Chemistry Education, Gyeongsang National University, Korea

[1]*Department of Chemistry Education, Gyeongsang National University, Korea*

Photo-Cleavable azo surfactants are utilized for protein extraction and subsequent mass spectrometry (MS) analysis. In the patent titled 'PHOTO-CLEAVABLE SURFACTANTS' (US Patent 11,567,085 B2, Jan 31, 2023) by Ying Ge et al., the authors elaborate that 4-hexylphenylazosulfonate effectively solubilizes proteins and peptide fragments with a performance level comparable to sodium dodecyl sulfate (SDS). They further suggest that it could serve as a viable substitute for SDS in gel electrophoresis applications.The photo-cleavable azo surfactant functions based on the principle of the degradation and decomposition of the azo moiety between the hydrophilic head and hydrophobic tail upon exposure to ultraviolet (UV) radiation. In this study, the introduction of various functional groups, including ether, ester, and amide, into the hydrophobic tail in addition to alkyl chains was undertaken to investigate the performance of these modified surfactants as interfacial agents. The synthesis of the photo-cleavable azo surfactant involves the conversion of primary amines via a diazo coupling reaction using sodium nitrite and hydrochloric acid, yielding diazonium salts. Subsequent reaction with sodium sulfite leads to the formation of the desired compound.

Poster Presentation : **ORGN.P-188**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Conjugatable Fluorophores with Ultralarge Stokes Shifts

Taehyeon Choi, Heechan Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Fluorescent labeling is a powerful non-destructive method for selectively detecting and identifying biomolecules. Fluorophores having large Stokes shifts are advantages as they suffer less from of detrimental self-absorption. To realize strong ESIPT emission with large Stokes shift, we devised molecular design strategies using *o*-phenylenediamine as a strong hydrogen bond donor. The corresponding hydrogen bonding acceptors are built with pyridine derivatives having systematically varied *para*-substituents, which provide significant thermodynamic stability to the proton-transferred(PT) tautomeric structure. We found that the emission from the PT state has a large Stokes shift of approximately 12,000 cm^{-1} and fluorescent quantum yield exceeding 20%. The absorption wavelength can be varied from 310 nm to 464 nm, depending on the electronic nature of the functional groups modifying the diamine unit. In addition, fluoropyridine derivatives facilitate the introduction of various nucleophiles through S_NAr reactions, and the ESIPT emission is maintained even in water. Our approach suggests the utility of these conjugatable fluorophores as protein markers. This presentation will discuss key design principles, synthetic implementations, and facile structural diversification into fluorophores libraries featuring large Stokes shifts.

Poster Presentation : **ORGN.P-189**

Organic Chemistry

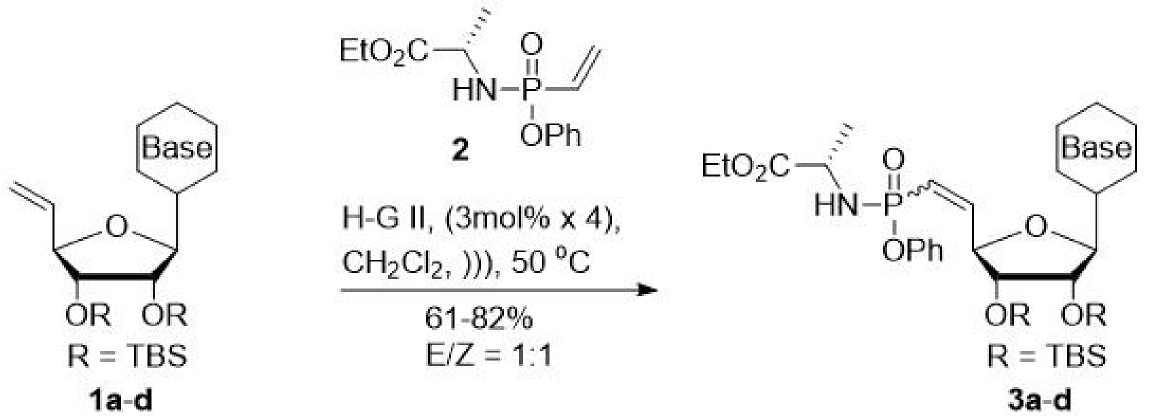
Exhibition Hall C FRI 11:00~13:00

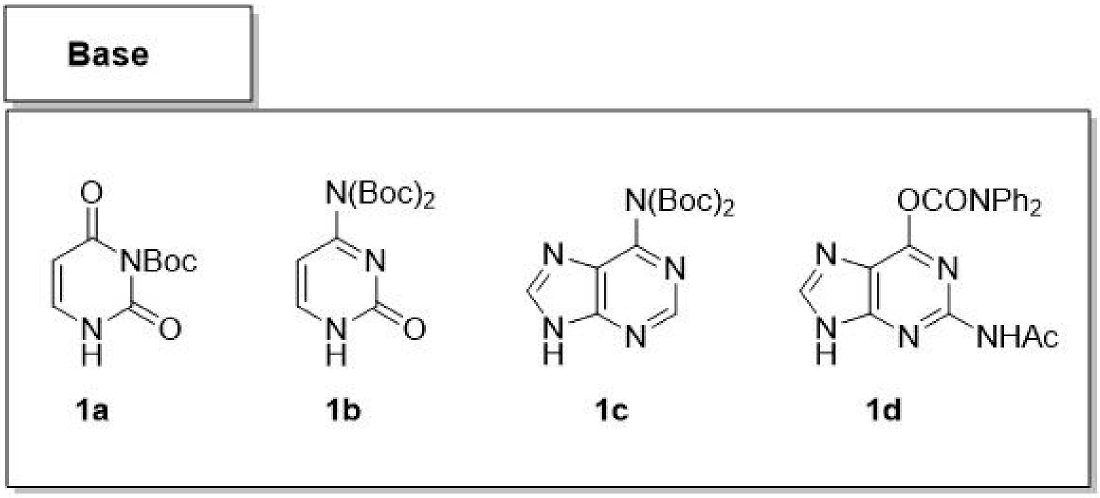
Efficient Synthesis of Nucleoside Phosphonamidate Prodrugs Using Cross Metathesis Associated with Ultrasonic Radiation

Se Myeong Choi, Yeon Jin An, Eun Rang Choi, Ji Yeon Yang, Yong Hun Choi, A Young Jung, So Jung Kwon, Jong Hyun Cho*

Department of Medicinal Biotechnology, Colleg of 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 and 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. Also, there is no approach for direct synthesis of nucleoside phosphonamidate derivatives using the cross metathesis (CM) to date. Herein, we present that a powerful tool for direct synthesis of vinylphosphonate/amidate derivatives and vinylfuranose analogs with CM reaction under the condition of a ultrasonic irradiation. With the optimal reaction condition of CM, the nucleotide phosphonate prodrugs (3a-d) (A, C, U, and G) were synthesized in 60-70% yield from the parent nucleoside analogs (1a-d).


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
O
NBoc
N
H
O
1a
N(Boc)2
N
N
H
O
1b
N(Boc)2
N
N
N
H
N
1c
OCONPh2
N
N
N
H
N
NHAc
1d

Poster Presentation : **ORGN.P-190**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Chiral Molecular Clips for Stereoselective Self-Assembly

<u>Sungryul Bae</u>, Dongwhan Lee[*]

Division of Chemistry, Seoul National University, Korea

In supramolecular chemistry, the control of assembly process is crucial. This task can be achieved by well-designed molecular building blocks with specific modes of interactions. Properly designed chiral molecules have the ability to differentiate between two enantiomeric forms. Such stereoselectivity is crucial for creating intricate functional structures, as seen in biological systems and asymmetric catalysts. We have explored the chemistry of letter C-shaped chiral molecular clips that are capable of stereoselective dimerization via hydrogen bonding and π–π stacking. A successful realization of the heterochiral dimerization of such molecules capitalizes on the shape complementarity of the building blocks. Chirality of the clips originate from the asymmetric spiro-junction of the linker that supports extended π-surfaces. This spatial orientation leads to the exclusive formation of heterochiral dimers by controlling the spatial positioning of the hydrogen bonding components. Experimental studies using ^{1}H-NMR spectroscopy on the solution samples revealed their strong preference for heterochiral dimers. Furthermore, X-ray crystallography analysis confirmed the heterochiral dimerization of mirror-image isomers of the clips in the solid-state. In the case of enantiopure clips, however, only weak homochiral dimerization is observed. Additionally, encapsulation of small polyheterocyclic guest molecules could compete with the dimerization process. This presentation will discuss the fundamental design principles governing the formation of chiral molecular clips, and future directions for creating diverse functional molecular architectures and their higher-order assemblies.

Poster Presentation : **ORGN.P-191**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

pH-Driven Hydrophobicity Switching for Anion Recognition in Water

Seungyeon Hyun, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Recognizing anions in water remains a significant challenge in supramolecular chemistry. The selective detection of hydrophobic anions, in particular, large, non-spherical, and charge-diffuse species, presents a significant challenge when relying solely on electrostatic interactions. We have developed multipodal cationic *N*-heterocyclic fluorophores for the recognition of hydrophobic anions in water by aggregation-induced emission (AIE). We demonstrated that changing the length of alkyl chains allows systematic modulation of the inherent hydrophobicity without electronically perturbing the light-emitting components. This structural modification aided selective detection of hydrophobic anions in water, as the degree of ion-pair aggregation depends on the hydrophobicity of both the cationic receptor and the anionic analyte. Building upon this concept, we further developed a series of water-soluble light-emitters that respond to two different types of stimuli. Functional groups installed at the terminal end of the alkyl pendant drive a large hydrophobicity change by protonation and deprotonation, thereby enabling pH-responsive anion detection. This presentation will discuss the key design principles, synthetic implementations, and practical applications of multi-podal and macrocycle-appended fluorophores for selective, sensitive and tunable recognition of ionic species in water.

Poster Presentation : **ORGN.P-192**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Photo-oxidation of 1,5-dihydroxynaphthalene (1,5-DHN) to 5-hydroxy-1,4-naphthalenedion (Juglone) slug based continuous flow system

Eung shin Lee

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

Recently, photo-oxidation using heterogeneous catalysts in continuous flow processes has been studied in various methods. In general, packed-bed systems and wall coating systems are used to apply heterogeneous catalysts, but these systems have several disadvantages such as clogging and difficult conditions. In this study, So we tryed to the slug flow system for photo-oxidation of 1,5-dihydroxynaphthalene (1,5-DHN) to 5-hydroxy-1,4-naphthalenedion (Juglone) in continuous flow. Juglone is used as a dye of cloth and ink, colorant of food and cosmetics and medically to treat various skin diseases, and is relatively expensive but difficult to supply on a large scale. Therefore, through experiments, juglone could be mass production under simple conditions as a slug flow system was applied in a continuous flow. Slug flow systems have the advantage of applying heterogeneous catalysts under simple conditions and making a uniform reactions for a long time with regular flows and droplet formation. The slug flow system is designed to disperse a heterogeneous catalysts in poly(ethylene glycol) (PEG) with high dispersion in silica gel, mixed it with the reactant, and then react while forming droplets with oxygen.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-193**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Photochemical reaction of intermolecular cyclization between N-((trimethylsilyl)methyl)-N-phenyl-substituted and N-phenylmaleimide via visible light

Hye Mi Yoo, Dae won Cho[1,*]

Yeungnam University, Korea

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

Stereoselective visible-light-driven annulation reaction between N-((trimethylsilyl)methyl)-N-phenyl-substituted and N-phenylmaleimide for the synthesis of substituted tetrahydroquinoline is presented.10 substrates were synthesized from ortho-alkylbenzaldehydes in a three-step procedure involving a carbonyl condensation, a radical bromination, and a substitution by a secondary α-silylmethyl amine.Then, by irradiating visible light, an intermolecular cyclization compounds were formed. The reaction conditions included the use of 5 mol% of a Methylene blue (MB) photoredox catalyst with MeOH as the solvent, under N_2-purged environment.Furthermore, various substrates were converted para position of phenyl ring of N-phenylmaleimide to make new compounds.The key point in this experiment is that the presence or absence of a silyl group is an important factor in cyclization formation.

Poster Presentation : **ORGN.P-194**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Modulating the frontier molecular orbitals of phenothiazine derivatives for electrochromic applications

Hyojin Cho, Young S. Park[*]

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

Electrochromic materials (ECMs) undergo a reversible color change caused by an electric current or potential. Compared to cathodic ECMs, there have been few studies on anodic ECMs. Herein, we introduce phenothiazine-based molecules that exhibit the characteristic of anodic coloration. By incorporating a phosphonic acid anchoring group, the molecules facilitate the formation of an organic-inorganic hybrid electrochromic film. By varying the substituents at the 3- and 7-positions of phenothiazine, we modulate the energy levels of the frontier molecular orbitals. The electrochromic device composed of MeO-2EPT, a methoxy-substituted phenothiazine derivative, leads to two consecutive redox reactions resulting in a color change, from transparent to greenish blue and then to blue. Notably, the device undergoes coloration and bleaching within 1 second. Furthermore, the first oxidation reveals an extremely high coloration efficiency of 470 cm^2/C. In addition, the long-term stability is demonstrated throughout 2,000 cycles. The reported findings may prove valuable for the development of anodic ECMs and the advancement of electrochromic technology.

Poster Presentation : **ORGN.P-195**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

The steric hindrance in PN annulation facilitated the synthesis of PN-fulvenes

Kim Hyunho, Young S. Park[1],*

Chemistry, UNIST, Korea

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

We describe a general method for synthesizing fulvene derivatives that contain a PN bond and elucidate the influence of steric hindrance on the formation of the exo-cyclic ring. Fulvenes, an isomer of benzene, are an interesting class of hydrocarbons consisting of cross-conjugated cyclic molecules. The synthesis detailed here is simple and provide the easy access to this interesting class of molecules. We have found that the steric hindrance induces the nucleophile-promoted electrophilic PN annulation, forming five-membered ring that is complementary to six-membered ring, previously reported by our group. We examine the PN annulation pathway by introducing different steric substituents on the nitrogen atom, using Taft parameters. Depending on the sterics on the nitrogen atom of 2-(phenylethynyl)aniline, 6-endo-dig PN annulation has shifted to 5-exo-dig annulation, resulting in PN-benzofulvene derivatives. Similarly, we explore the electronic effect on phenyl groups in PN annulation by substituents; however, we are unable to achieve a conversion of the reaction pathway. The prepared PN-fulvenes are characterized by X-ray crystallography, NMR spectroscopy, UV-vis spectroscopy, and cyclic voltammetry. Finally, the regiochemistry of the 5-exo-dig product is determined to be the E isomer by NOESY.

Poster Presentation : **ORGN.P-196**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Cu-Catalyzed Regioselective Hydrosilylation of Mono- and Di-substituted Allenes

Yurim Lee, Min Kim, Yunmi Lee[1,*], Byunghyuck Jung[2,*]

Physics & Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*
[2]*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Allylsilanes are used in a wide range of fields such as biochemistry, pharmaceuticals, and industrial materials as well as useful synthetic building blocks in organic synthesis. Although many synthetic protocols of preparing allylsilanes have been reported so far, synthetic approaches through transition-metal catalyzed regioselective hydrosilylation of allenes are few owing to the difficult control of regio- and stereoselectivity. Especially, protosilylation strategies, which use acidic protons as H source (i.e. RO-H) rather than hydrides such as H-Si, H-B, or metal hydrides for general hydrosilylation, are very rare. Herein, we present regioselective synthesis of linear allylsilanes from mono- or 1,1-disubstituted allenes through Cu-catalysis. In our synthetic method, both simple alkyl-substituted allenes and tertiary 2,3-allenols produced the desired linear products in high yields and regioselectivity. In addition, 1,1-disubstituted allenes have broad scopes of substrates such as exo-cyclic allenes, alkyl/alkyl, and aryl/alkyl-substituted allenes in good yields with excellent regioselectivity. Our protocol also showed the high functional group tolerance. Finally, we demonstrated Lewis-acid catalyzed stereoselective allylation to carbonyls to verify their synthetic utilities. Now, we are pursuing to unveil the reaction mechanism by experimental and computational studies.


R1
R2
1
2
3
Cu
PhMe2SiBpin
additives, RT, 6 h
SiMe2Ph

Poster Presentation : **ORGN.P-197**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Protocatechuic acid derivatives effectively inhibit TNF-α-induced inflammatory response.

Yunseul Park, Se Won Bae[1,*], Jaehoon Cho[2,*]

Jeju National University, Korea
[1]*Department of Chemistry, Jeju National University, Korea*
[2]*Korea Institute of Industrial Technology, Korea*

The immune response is a biological process that occurs through complex chemical interactions involving multiple stages and molecules. The skin plays a vital role in defending against various stimuli from the external environment. Inflammatory skin disorders begin with an increased expression of molecules such as cytokines, interferons, and interleukins, leading to the activation of the immune system. The tumor necrosis factor alpha (TNF-a) induced inflammatory response in the skin can lead to conditions like dermatitis and even affect melanin production.Protocatechuic acid (PCA), a phenolic compound derived from plants, possesses various pharmacological activities including anti-inflammatory, antioxidant, and anticancer effects. It holds protective effects against the development of inflammatory skin conditions and epithelial malignancies within our tissues. The mechanism of this action is predominantly associated with antioxidant activities, encompassing the inhibition and elimination of free radical generation.In this study, PCA derivatives were synthesized to produce effective anti-inflammatory compounds. We hypothesized that our synthesized derivatives would more effectively suppress TNF-a induced inflammatory responses compared to PCA alone. We verified this by conducting enzyme-linked immunosorbent assays (ELISA) to confirm the effect. Additionally, we performed MTT experiments to assess cell viability influenced by PCA derivatives.The results revealed that our synthesized PCA derivative compounds more effectively inhibit TNF-a induced inflammatory responses than PCA alone. The PCA derivatives, coupled with alkyl esters, may be suitable for inclusion in skincare product formulations, given their potential benefits in skin health and inflammation management


사단법인 대한화학회
KOREAN CHEMICAL SOCIETY

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-198**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Fluorescent tagging of proteins using flow chemistry

<u>Heejoo Shin</u>, Se Won Bae*

Department of Chemistry, Jeju National University, Korea

Conventional protein fluorescence tagging methods have been performed as batch processes. A batch process is a chemical reaction in which all the reactants are placed into a reaction vessel at once using a fixed amount of material for a specific period of time, and the reaction proceeds to completion. However, in this batch process, the reaction conditions undergo changes during the reaction time, leading to inconsistent reaction outcomes. This inconsistency makes it challenging to control the reproducibility of the reaction product. Flow chemistry is attracting attention as an alternative that can solve these problems of existing batch chemistry. Flow chemistry involves continuous chemical reactions within a flowing fluid. This approach offers several advantages, including more precise control of chemical reactions, the facilitation of scale-up and automated processes and improving the reproducibility of reaction products.We have developed a method for selectively attaching fluorophore (FITC) to lysine residues in peptides and controlling the quantity of FITC molecules reacting with the residues based on flow chemistry. Through this process, the number of FITC attached to lysine residues can be regulated based on the residence time in the flow reactor. Furthermore, by implementing an automated process, the yield can be further enhanced through continuous reactions in the flowing fluid. In conclusion, our new bioconjugation method through flow chemistry is expected to play a very important role in related field in the future.

Poster Presentation : **ORGN.P-199**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Efficient Detection of Heavy Metal Lead Ions in Water using AIE-based Turn-on Fluorescence Sensor

Haemin Choi, Hyeonjeong Seong, Juyeon Cha[1], Seoung Ho Lee[2,*]

Department Chemistry, Daegu University, Korea

[1]*Department of Cosmetics & Bioscience, Daegu University, Korea*

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

Lead, a heavy metal widely employed in various industries, continues to pose a threat to both human health and the environment. Therefore, the development of a sensor capable of rapidly and accurately detecting lead(II) ions in real-time at contaminated sites is crucial. In this study, we have engineered a fluorescent sensor with the ability to efficiently detect lead(II) ions in actual environmental conditions, including tap water and freshwater. The compound TPE-COOH exhibits high selectivity and sensitivity towards lead(II) ions, leading to a fluorescence increase upon interaction between compound TPE-COOH and lead(II) ions. Impressively, compound TPE-COOH proficiently detects lead(II) ions in tap water and freshwater, even in the presence of various interfering substances.

Poster Presentation : **ORGN.P-200**

Organic Chemistry

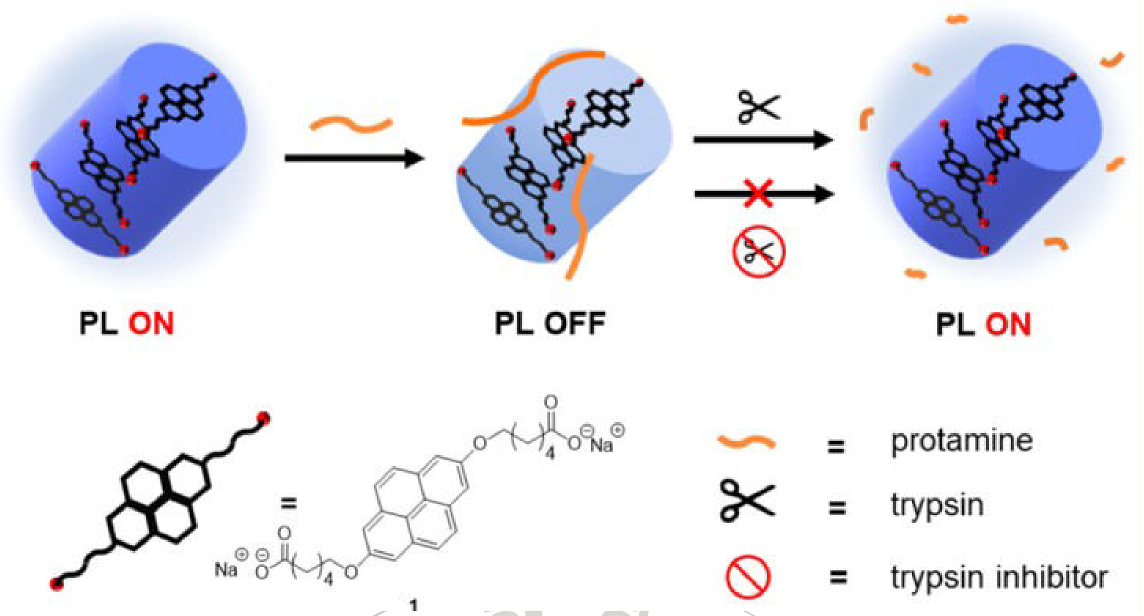
Exhibition Hall C FRI 11:00~13:00

Ultrasensitive Determination of Trypsin in Human Urine Based on Amplified Fluorescence Response

Minwoo Han, JaeMin Lim, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

The determination of trypsin activity in human urine is important for evaluating pancreatic disease. We designed an effective fluorescence sensing strategy based on a self-assembled amphiphilic pyrene/protamine complex system that provides an amplified fluorescence response for highly sensitive and selective detection of trypsin. In aqueous solution, the functionalized pyrene formed fluorescent, π-extended aggregates inside micelles, which were effectively quenched by protamine (a trypsin substrate). However, this quenched fluorescence was very sensitively recovered by the trypsin's enzymatic reaction, and this was attributed to a marked reduction in enhanced exciton migration caused by protamine in π-delocalized pyrene aggregates. The devised sensing platform was successfully utilized to selectively and sensitively detect trypsin at very low concentrations (0.03−0.5 μg mL−1) in non-pretreated human urine and to screen for trypsin inhibitors at concentrations of 0.1−5.0 μg mL−1.



PL ON
PL OFF
PL ON
=
Na
O
O
4
O
O
4
O
Na
1
= protamine
= trypsin
= trypsin inhibitor

Poster Presentation : **ORGN.P-201**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Ratiometric Fluorescence Detection of Tyrosinase Activity Based on Excited-State Proton Transfer

Minwoo Han, Haemin Choi[1], Seoung Ho Lee[*]

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

Tyrosinase plays a crucial role in melanin synthesis and serves as a significant biomarker for melanoma. To date, various methods such as quantum dots, colorimetric, and fluorogenic turn-on/off techniques have been employed in prior studies to detect tyrosinase activity. However, these approaches exhibit limitations in terms of sensitivity and reliability. In this study, we have designed and synthesized a novel probe capable of facilitating ratiometric fluorescence measurement through excited-state proton transfer (ESPT). The probe demonstrates a distinct blue fluorescence emission, and its 3-hydroxyphenyl moiety undergoes reduction to the o-quinone form via an enzymatic reaction with tyrosinase. Through the implementation of this ratiometric strategy, we have effectively demonstrated the sensitive and selective detection of tyrosinase. Additionally, this approach enables the screening of tyrosinase inhibitors, which are of paramount importance in preventing severe skin conditions, developing skin whitening products, and mitigating browning in fruits.

Poster Presentation : **ORGN.P-202**

Organic Chemistry

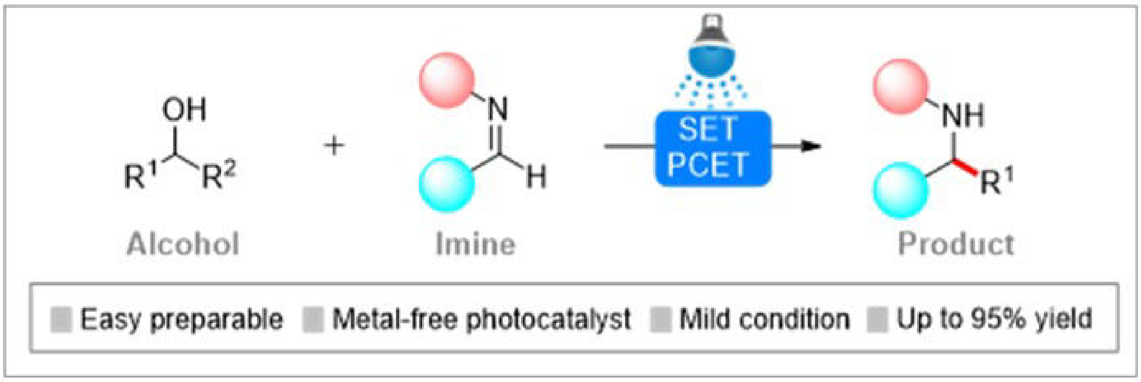
Exhibition Hall C FRI 11:00~13:00

Visible-Light-Mediated Alkylation of Imines Using Alcohol as a Radical Precursor

Jae young Kim, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

Imines are important intermediates in the synthesis of amine scaffolds. The amines are widely used as feedstock chemicals and building blocks for biologically active compounds in agrochemicals and pharmaceuticals. Traditionally, amines are synthesized by imine addition reactions using organometallics as nucleophiles. In the past decade, visible light photoredox-catalyzed imine addition reactions have been developed to prepare amines using various radical precursors, such as alkyl trifluoroborates and silicates. Herein, we report a new strategy for the synthesis of amines using alcohols as alkyl radical precursors via the PCET mechanism under photoredox catalysis. A wide range of alkyl amines were obtained in good to excellent yields. This strategy was also conducted under mild conditions using a metal-free photocatalyst.



Poster Presentation : **ORGN.P-203**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Monomeric Masked ortho-Benzoquinones via Oxidative Dearomatization of ortho-Substituted Phenol MIDA Boronates

Taelyn Kim, Jimin Lee, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Oxidative dearomatization of ortho-substituted phenols has been widely utilized to prepare linearly conjugated cyclohexa-2,4-dienones. Due to the ketal protection of one carbonyl group in ortho-benzoquinone, these compounds have been also known as masked ortho-benzoquinones (MOBs). MOBs have been considered important in organic synthesis because they can be utilized as key intermediates in various organic reactions. Despite their synthetic utilities, application of the MOBs to natural product synthesis has been very limited due to formation of MOB dimer through Diels-Alder reaction. Therefore, the development of a protocol to access a monomeric MOB has considered the research of importance, and several methods have been developed through suppressing MOBs homo-dimerization by the careful control of the electronic nature or steric hindrance of substituents on the phenol ring. However, no general method for forming monomeric MOB has been developed so far. In this poster presentation, we disclose the development of a new synthetic method to form masked ortho-benzoquinones (MOBs) in monomeric form through oxidative dearomatization of ortho-substituted phenol MIDA boronates using the MIDA group as a blocking group for dimerization. Furthermore, the application of the resulting MOBs in various organic transformations would be presented.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-204**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Skeleton Divergent Total Synthesis of Monoterpene Indole Alkaloids

Myunghoon Jeong, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Monoterpene indole alkaloids are a diverse class of natural products, comprising over 2000 members. These complex natural products exhibit a wide array of chemical structures and encompass a wealth of biological activities. Hirsutine, ajmalicine, and yohimbine, despite sharing structural similarities as Corynanthe-type alkaloids, have each followed distinct synthetic pathways. In this poster presentation, we disclose a skeleton-divergent total synthesis of several indole monoterpene alkaloids bearing a structural similarity. We intend to present the retrosynthetic analysis and total synthesis 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-205**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthetic Studies towards Guettardine

Seungmin Ryu, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Guettardine was first isolated and identified in 1984 from the bark of Guettarda heterosepala. Guettardine is one of notable indole alkaloids due to its role which represents an important link in the synthesis of the corynanthe–cinchona alkaloids, Further, guettardine possesses diverse pharmacological and biological properties. Structurally, guettardine features a tryptophol framework bearing N-methyl-piperidine motif with three stereogenic centers. The first and only total synthesis of guettardine have been accomplished by the group of Rubiralta in 1990. Imine formation of indole-2-carboxaldehyde derivative and primary amine, and Mannich-type cyclization was used to make core structure. That process led to epimerization, yielding 15-epiguettardine as a byproduct. Also, the previous synthesis has utilized primary amine to synthesize piperidine scaffold, which required lengthy synthetic sequence.In this poster, we present the synthetic studies toward guettardine. The cyanide-catalyzed imino-Stetter reaction of 2-aminocinnamate and acetal-protected 5-acetylpicolinaldehyde was used to prepare 2-piperidine substituted indole derivative as core unit. Pyridinium reduction was selected to prepare piperidine ring in this protocol. Michael addition is used to control two stereogenic centers of piperidine scaffold. Further studies will be needed to control stereocenter in piperidine ring.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-206**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of 3-trifluoromethyl benzo[b]thiophenes via electrochemical cyclization reaction

Gihun Kwak

Korea Research Institute of Chemical Technology, Korea

Benzo[b]thiophenes are essential structure motifs and are widely presented in a great number of biologically active compounds and natural products. As a consequence, considerable effort has been made to develop efficient strategies for the construction of benzo[b]thiophene such as transition metal catalyzed cyclization, halogen mediated cyclization, and radical reaction. However, available methods for the synthesis of trifluoromethylated benzo[b]thiophenes are very limited, which has hampered the biological studies of such an important class of trifluoromethylated heterocycles. Fortunately, a number of trifluoromethylation reactions of unsaturated C-C bonds have been reported since CF3 radicals can be effectively generated through an electrochemical redox reaction. Therefore, we attempted to synthesize 3-trifluoromethyl benzo[b]thiophene via cyclization reaction using the electrochemically generated CF3 radical. The details of the study will be described in this presentation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-207**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Characterization of selenium-containing non-fullerene acceptors for organic solar cells

Hye Yeon Park, Yun Hi Kim[1,*]

Materials Engineering and Convergence Technology, Gyeongsang National University, Korea
[1]Department of Chemistry, Gyeongsang National University, Korea

Non-fullerene acceptors (NFAs) have been crucial in improving the efficiency of organic solar cells (OSCs) due to their attractive properties, such as strong light-harvesting ability, easily tunable energy levels, and high crystallinity. Nevertheless, general NFAs have limited light absorption, and studies on the design of NFAs that can absorb a broad range of the solar spectrum and that have absorption complementary to that of donors should be conducted. Because selenium can induce strong intermolecular Se···Se interactions, planarity, and extended effective conjugated length in OSC materials, in our study, we synthesized a series of selenium-substituted Y6 derivatives with different inner alkyl chain lengths, Se-Y6- BO and Se-Y6-HD. The optical absorption of two selenium-containing NFAs was redshifted compared with that of Y6 due to the effect of selenium atoms in the backbone.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-208**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Alkaline phosphatase responsive disulfide formation for transforming into fiber structure inside mitochondria of senescent cells

Sangpil Kim, Ja-Hyoung Ryu[1,*]

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

The intracellular biomacromolecules including proteins, DNA, and polysaccharides, play an important role to perform cellular function. Theses macromolecules have specific structure synthesized by the self-assembly of small molecules such as amino acids, nucleotides, and monossacharides, but they have distinct properties that the small molecules do not have. Interestingly, the structure could be transformed into two or more alternative conformations under a given environment, which is related to multiple physiological activities of biological entities. From this perspective, understanding the mechanism of structural transformation could open a new chapter to explore artificial chemical system that imitates bioprocesses. Herein, we developed intracellular transformable assembly system via disulfide formation, in which the spherical structure (inactive form) would be transformed into the fiber structure (active form) for regulating cellular fate. The designed monomer, in which the thiol groups were blocked by phosphate groups, did not form a disulfide bond and assembled into a spherical structure in a zwitterionic form. The p-Mito-1 undergoes rapid dephosphorylation catalyzed by ALP to form Mito-1, thereby accumulating into mitochondria and transforming into fiber structure through disulfide formation by reactive oxygen species (ROS). The resulting fiber structure disrupted the mitochondrial membrane, leading to activation of apoptotic signaling toward senescent cell.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

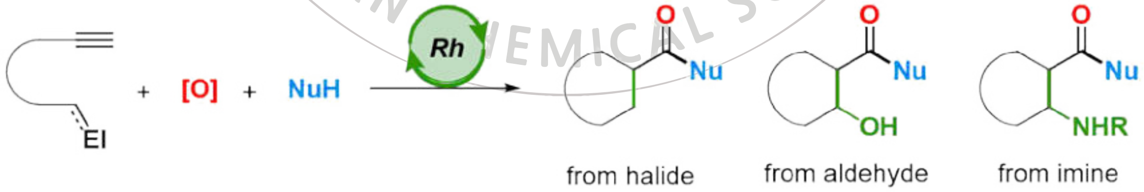
Poster Presentation : **ORGN.P-209**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Carbofunctionalization of Terminal Alkynes via Combined Rhodium Catalysis Enabling Formations of Four Different Bonds

<u>Dae-Kwon Kim</u>, Minjung Keum, Chulbom Lee*

Division of Chemistry, Seoul National University, Korea

Described here is the oxygenative carbofunctionalization of terminal alkynes mediated by combined rhodium catalysis that enables regioselective quadruple formation of C–C, C–H, C–O, and C–heteroatom bonds. Mechanistic studies suggest that a disubstituted rhodium vinylidene complex is generated upon C–C bond formation at the terminal alkyne with tethered electrophiles such as alkyl halides, aldehydes, imines, and Michael acceptors. Subsequent intermolecular transfer oxygenation of the rhodium vinylidene with pyridine N-oxide generates a rhodium-complexed ketene intermediate that reacts with a variety of heteroatom nucleophiles to give rise to cyclic carboxylic acid derivatives.



Poster Presentation : **ORGN.P-210**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Supramolecular Polymerization of *p*-phenylene Linked Metalloporphyrin Dyads

Yongho Lee, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Supramolecular polymers have received increasing attention in materials science due to their fascinating structures and unique functions. As an efficient method to construct well-defined nanoarchitectures, the field of supramolecular polymers provides new paradigms in materials design from a different perspective than conventional polymers. Here, we designed a range of metalloporphyrin dyads (specifically $^{D}PD_{M}$, $^{T}PD_{M}$ with M being Zn or Cu) connected through a *p*-phenylene linkage as monomeric building blocks for supramolecular polymers. To explore distinct self-assembled structures upon the substituents and central metal atom on the porphyrin units, temperature-induced supramolecular polymerization was conducted and monitored by UV-Vis spectroscopy. Through a gradual cooling process, both $^{D}PD_{Zn}$ and $^{T}PD_{Zn}$ showed bathochromic shifted absorption band, indicating the J-type stacking of porphyrin aggregates. Also, the formation of spherical nanoparicle assemblies was observed by atomic force microscopy (AFM). On the contrary, porphyrin dyads containing another metal displayed the distinct behavior. $^{D}PD_{Cu}$ showed hypsochromic shifted absorption band in the same cooling process, indicating H-type stacking of porphyrin aggregates. It was observed that helical nano-sized fibrous aggregates were formed. $^{T}PD_{Cu}$ exhibited its own distinct pattern of aggregation with a hyperchromic shift in the absorption spectrum over the cooling process. Furthermore, we were able to trace the supramolecular polymerization mechanism for each of these assemblies through spectroscopic studies.

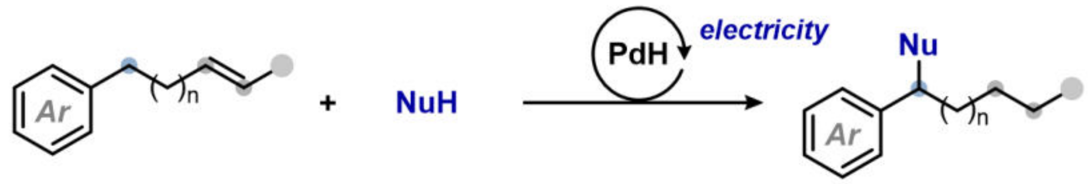
Poster Presentation : **ORGN.P-211**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Electrooxidative Palladium-Catalyzed Remote Hydrofunctionalization of Olefins with Nucleophiles

Seungdae Park, Baeho Yang, Dohyun Lee, Hyunwoo Kim[1,*], Kwangmin Shin[*]

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

The development of catalytic methods for the selective installation of carbon-carbon or carbon-heteroatom bonds into desired molecules has been regarded as a pivotal goal in modern organic chemistry. Among the developed synthetic strategies, remote hydrofunctionalization of olefins via chain-walking has recently emerged as a promising approach to achieve regioselectivity that is otherwise challenging to achieve through the conventional methods. This strategy has been successfully employed to achieve remote C-C, C-B, C-N, and C-S bond formation reactions. However, while the use of electrophilic reagents has been widely investigated, the development of a catalytic method for constructing carbon-heteroatom bonds employing nucleophiles as viable coupling partners has been significantly limited, likely due to the challenges in finding a compatible oxidation system. Herein, we report that the merger of palladium catalysis with electrooxidation, a controllable and compatible oxidation method, allows remote hydrofunctionalization of olefins with a variety of nucleophiles, such as alcohols, water, phenols, carboxylic acids, aniline, sulfonamide, carbamate, urea, and the HF reagents. A series of control and mechanistic studies suggest that the fast and uni-directional chain-walking followed by the generation of a high-valent palladium intermediate via anodic oxidation is the key step in this transformation.



nucleophile (**NuH**) = alcohols, water, phenols, carboxylic acids (***O*-nucleophiles**)
aniline, sulfonamide, carbamate, urea (***N*-nucleophiles**)
$Et_3N \cdot 3HF$ (***F*-nucleophile**)

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-212**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

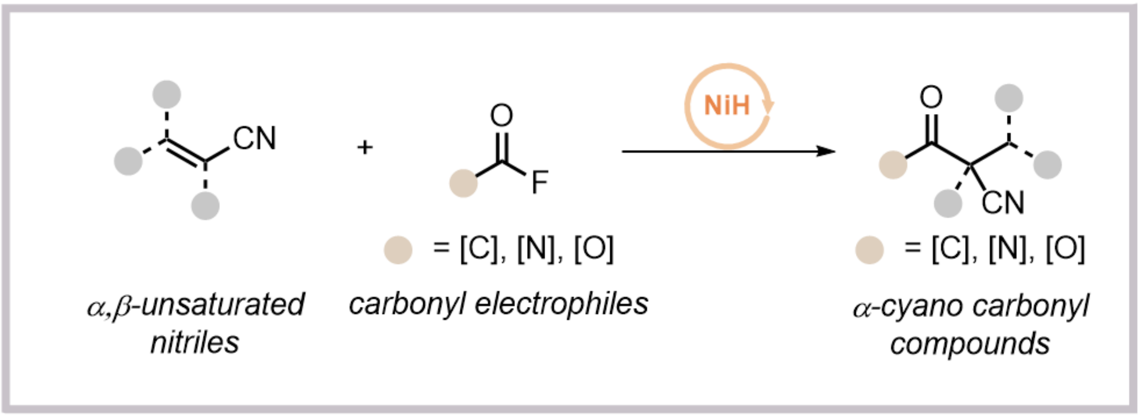
General access to α-cyano carbonyl compounds via NiH-catalyzed hydrofunctionalization of α,β-unsaturated nitriles with carbonyl electrophiles

Yoonho Lee, Yujin Jung, Kwangmin Shin[1,*]

Department of chemistry, Sungkyunkwan University, Korea

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

α-Cyano carbonyl compounds are important structural units prevalent in pharmaceuticals and biologically active molecules. Moreover, these structures are recognized as valuable building blocks in organic synthesis. As a result, various approaches have been developed to prepare α-cyano carbonyl compounds. However, (transition) metal-hydride catalyzed hydrofunctionalization of α,β-unsaturated nitriles with carbonyl electrophiles, another appealing and efficient synthetic strategy, has rarely been explored. Herein, we report a nickel-hydride-catalyzed hydrofunctionalization of α,β-unsaturated nitriles with acyl fluorides, carbamoyl fluorides, and fluoroformates. This method facilitates the synthesis of both tertiary and challenging quaternary carbon-centered α-cyano carbonyl compounds.



Poster Presentation : **ORGN.P-213**

Organic Chemistry

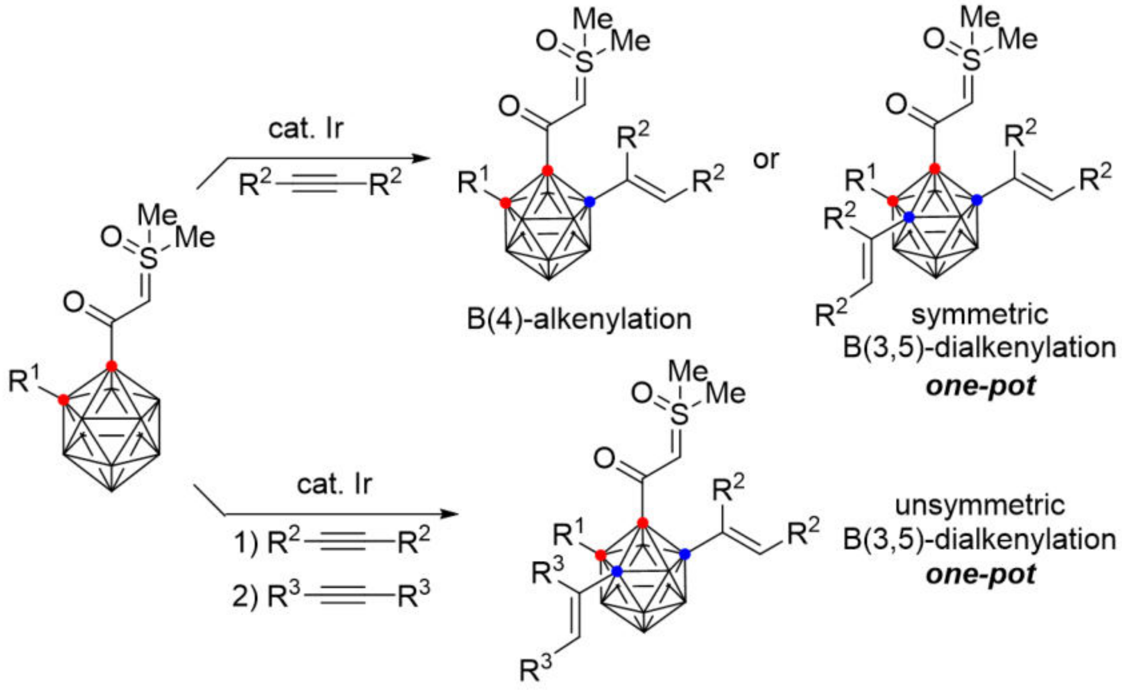
Exhibition Hall C FRI 11:00~13:00

Iridium-Catalyzed Regioselective B(4)-Alkenylation and B(3,5)-Dialkenylation of *o*-carboranes

Jiwon Kim, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

Iridium(I)-catalyzed regioselective B(4)-alkenylation has been developed from o-carboranyl sulfoxonium ylides and alkynes through B(4)−H activation. The sequential B(4)- and B(6)-alkenylation afforded B(3,5)-dialkenylated *o*-carboranyl sulfoxonium ylides in one pot. Eventually, two alkenyl groups, the same or different, were introduced at positions 3 and 5 of the carborane. Sulfoxonium ylide used as a directing group remains available for further functionalization and is converted to B-alkenylated *o*-carboranyl trichloromethyl ketones.


cat. Ir
R^2—≡—R^2
or
B(4)-alkenylation
symmetric
B(3,5)-dialkenylation
one-pot
cat. Ir
1) R^2—≡—R^2
2) R^3—≡—R^3
unsymmetric
B(3,5)-dialkenylation
one-pot
R^1
R^2
R^3
O
Me
S

Poster Presentation : **ORGN.P-214**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

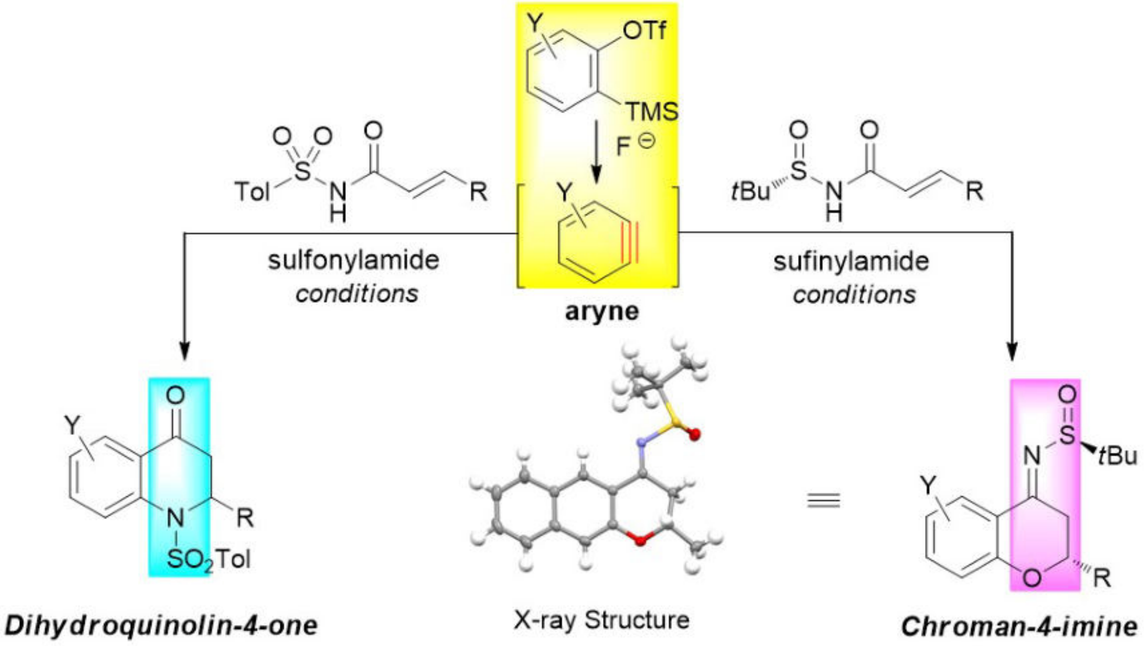
Conversions of Sulfonylamides and Sulfinylamides with Benzyne Intermediates for the Selective Formation of Dihydroquinolin-4-one and Chroman-4-imine Skeletons

Jihye Lee, Zhang Aimin, Seojung Han[1], Jimin Kim[*]

Department of Chemistry, Chonnam National University, Korea

[1]*Chemical and Biological Integrative Research Center, Korea Institute of Science and Technology, Korea*

Benzyne species are geometrically highly strained and kinetically reactive intermediates, which are recognized as valuable active species from an synthetic point of view in the production of useful chemical architectures. Various chemical transformations involving the use of benzyne intermediates have been developed in the construction of useful natural and unnatural substances. We present herein control factors for a general and efficient method of the reaction from benzyne intermediates to regulate the regiochemical routes with high levels of regio- and stereoselectivity. We also discuss scope and limitation of this unprecedented transformation and mechanistic details for stereoselectivity . In addition, synthetic applications can be foreseen for the products to give a variety of bioactive natural products.


Y
OTf
TMS
F ⊖
Y
aryne
Tol
S
N
H
R
sulfonylamide
conditions
tBu
S
N
H
R
sufinylamide
conditions
O
Y
N
R
SO₂Tol
Dihydroquinolin-4-one
X-ray Structure
O
S
N
tBu
Y
O
R
Chroman-4-imine

Poster Presentation : **ORGN.P-215**

Organic Chemistry

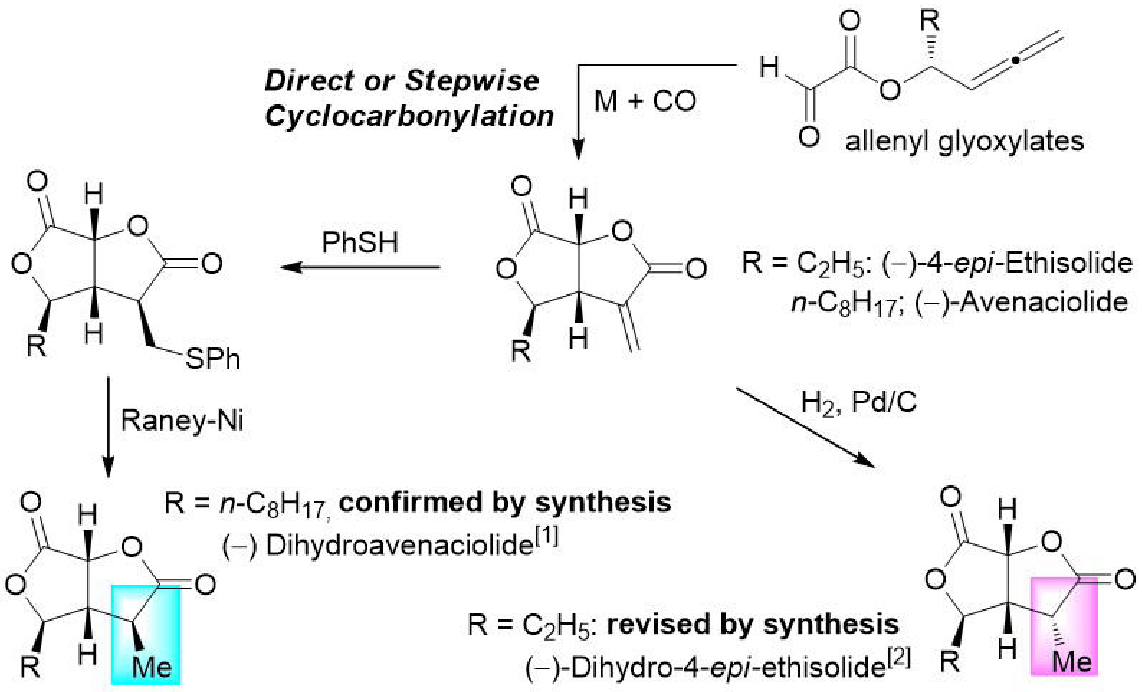
Exhibition Hall C FRI 11:00~13:00

Synthesis of Naturally Occurring Dihydroavenaciolide and Dihydro-4-epi-ethisolide through Cyclocarbonylation of Allenyl Glyoxylate: Correction of Stereochemistry

Jisu Kim, Suh Young Yu, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Dihydroavenaciolide and dihydro-4-epi-ethisolide were isolated from endophytic fungus species. The structural elucidations of both natural products were authenticated by nuclear magnetic resonance, especially NOE experiments. However, we realized that there are some ambiguity to determine relative stereochemistry at C-3 position according to the molecular model studies. The structural assignment of many of natural products has come primarily from NMR experiments with single crystal X-ray diffraction being used where possible. The unambiguous assignment of natural products structures with compounds not suitable for single crystal X-ray analysis is a challenging task and it is inevitable that incorrect structures are reported in the literature with these structural misassignments frequently being uncovered through synthesis. We present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring dihydroavenaciolide family: i. enantioselective synthesis of precursors avenaciolide and 4-epi-ethisolide from allenyl glyoxylates via a cyclocarbonylation; ii. synthesis of both epimers at C-3 position; iii. unambiguously reassigned or confirmed stereochemical relationship.



[1] Wu, S.-H. et al. *J. Am. Chem. Soc.* **2015**, *137*, 267.
[2] Ali, A. et al. *Med. Chem. Res.* **2017**, DOI 10.1007/s00044-017-1989-4

Poster Presentation : **ORGN.P-216**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

MOF-TEMPO-Catalyzed Oxidative Cyclization Between Aminophenol and Aldehydes

Jonghyeon Lee, Daeyeon Lee, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs) are highly crystalline and porous materials, which are constructed by coordination bonding between metal cluster and organic ligands. By attaching a variety of catalytic species to the pores and framework of the MOFs, the MOFs can be used as heterogeneous catalysts.[1]

Here in, we present that our recent stuty for the catalytic applications of TEMPO radical-functionalized MOFs toward benzoxazole synthesis. Previously, MOF-TEMPOs were succesfully applied to heterogeneous aerobic oxidations of alcohols.[2] The unique oxidation ability of MOF-TEMPO then applied to oxidative cylcization between aminophenols and aldehydes to form benzoxazole derivatives. The optimization of the reaction, as well as the substrate scopes will be present in the presentation.

References

1. Lee, J.; Hong, S.; Lee, J.; Kim, S.; Kim, J.; Kim, M. *Bull. Kor. Chem. Soc.* **2021**, *42*, 359-368.

2. Lee, J.; Hong, S.; Heo, Y.; Kang, H.; Kim, M. *Dalton Trans.* **2021**, *50*, 14081-14090.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-217**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Amine Functionalizations on Dopamine Molecules

Yoonji Heo, Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea

Dopamine molecule has both acidic catechol and basic aliphatic amine groups in their molecular structure. Not only for their neurobiological properties, but also their polymeric aggregations have been widely applied to surface-coating and modification of various solid materials. The structural modifications of dopamines have been studied.[1]

In this presentation, our recent efforts for amine modification in dopamine will be discussed. Based on our recent study about dopamine methylation,[2] we have introduced additional alkyl chains on amino group of dopamine. In addition, further functionalization on amine group of dopamines have been performed. The detail synthesis and characterization along with polydopamine expriments will be discussed in the presentation.

References

1. Liebscher, J. *Eur. J. Org. Chem.* **2019**, 4976.

2. Kim, Y.; You, A.; Kim, D.; Bisht, H.; Heo, Y.; Hong, D.; Kim, M.; Kang, S. *Langmuir*, 2022, *38*, 6404.

Poster Presentation : **ORGN.P-218**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Background-Signal-Minimized Fluorescent Sensing Systems for Alzheimer's Diseases Diagnosis

Soyeon Yoo[*], Gyo chang Keum, Min Su Han[1,*], Eun-Kyoung Bang[*]

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

Alzheimer's disease, one of the neurodegenerative diseases, is rapidly increasing in current society, and early diagnosis is of paramount importance due to the difficulty in recovering once brain cells are damaged. Major biomarkers include amyloid beta (Aβ) and tau aggregates. Additionally, butyrylcholinesterase (BchE), an enzyme that hydrolyzes choline-based esters like the neurotransmitter acetylcholine, is emerging as a potential biomarker due to its increased activity in the brains of Alzheimer's patients. The inhibitor of this enzyme has been actively studied as a potential treatment for Alzheimer's disease. Fluorescent-based sensing systems offer advantages such as high sensitivity, non-destructiveness, and real-time analysis, making them suitable for high-throughput screening (HTS) of inhibitor candidates for biomarkers as well as detecting biomarkers. However, high selective and quantitative detection of target biomarkers is challenging due to issues such as auto-fluorescence, high non-specific binding affinity to fluorescent probes of human serum albumin (HSA) that is present in excess in the blood, and interference with similar biomaterials. Therefore, reducing the background signal caused by these obstacles is crucial in developing effective fluorescent sensors.To address the non-specific fluorescence resulting from the non-specific binding of HSA to fluorescent probes, we utilized this non-specific fluorescence in reverse as part of the sensing system. A novel fluorescent sensing system for the detection of BchE was devised using HSA and a caged form of the probe with strong fluorescence upon binding to HSA. After the caged probe was de-caged by hydrolysis of BchE, the probe bound to HSA and emitted strong fluorescence. This system allowed accurate quantification of BchE activity present in actual human serum by simply adding the probe to the serum, utilizing the HSA already present

in the sample. This approach was also applicable to HTS for BchE inhibitors.To overcome interference with similar biomaterials and auto-fluorescence, we developed a red-fluorescent probe sensitive to Aβ aggregates. The probe had a dipolar structure with a donor(D)-π-acceptor(A) configuration. Inspired by the structures of [F-18]FDDNP and Thioflavin T, known to have high binding affinity to Aβ, we introduced 6-(dimethylamino)naphthalene and benzothiazole as the D and A moieties. We optimized the distance between D and A based on the following research findings: (1) a distance of less than 13 Å is highly selective for Aβ over tau, and (2) longer π-conjugation induces a red-shift in the emission wavelength. The devised probe exhibited red fluorescence with minimal autofluorescence interference and high selectivity for Aβ over Tau and albumins. Furthermore, it was used for ex vivo fluorescence imaging of Aβ aggregates present in the brains of mice with Alzheimer's disease.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-219**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Chemodynamic/Photodynamic Synergistic Therapy for Cancer Stem Cell with A Carbonic Anhydrase IX-targeted Cu(II)-BODIPY PS complex

<u>Eunbin Hwang</u>, Jungmin Lee[1], Lee Soeun[2], Seyoung Koo[3], Miae Won[4], Jong Seung Kim[5,*], Hyo Sung Jung[6,*]

Department of Gerontology(AgeTech-Service Convergence Major), Kyung Hee University, Korea
[1]*thishand01@naver.com, Department of Biomedical & Chemical Sciences, Korea*
[2]*Department of Biomedical & Chemical Sciences, thishand01@naver.com, Korea*
[3]*Department of Chemistry, Hyupsung University, Korea*
[4]*R&D institute, TheranoChem Inc., Korea*
[5]*Department of Chemistry, Korea University, Korea*
[6]*Department of Biomedical & Chemical Sciences, Hyupsung University, Korea*

Among the various emerging cancer-treatment strategies, photodynamic therapy is attractive as a potentially less invasive modality than other treatments, such as surgery, chemotherapy, and radiotherapy. To date, a number of photosensitizers have been developed for treating cancer, and more recently, advanced organic photosensitizers have attracted significant attention as potential complementary tools or alternatives to classical sensitizers or anticancer agents.In this poster presentation, I will discuss the development of organic–metal chemo/photosensitizers for cancer stem cell (CSC) treatment. Chemoresistance originating from CSCs is a major cause of cancer-treatment failure and necessitates the need to develop effective CSC-targeting therapies. Although significant progress has been made in both PDT and chemodynamic therapy (CDT) in recent decades, the efficacies of these modalities against CSC remains limited. Therefore, we developed a new-generation photosensitizer, denoted as CA9-BPS-Cu(II), a system that combines three subunits within a single molecule, viz., a copper catalyst for CDT, a boron dipyrromethene photosensitizer for PDT, and acetazolamide for targeting CSC via CAIX binding. We

observed a therapeutic effect in MDA-MB-231 cells, attributable to elevated oxidative stress mediated by a combined CDT/PDT effect, as well as copper-catalyzed glutathione oxidation. The CSC-targeting ability of CA9-BPS-Cu(II) was evident from its specific affinity to CD133-positive MDA-MB-231 cells. Moreover, its efficacy was successfully demonstrated in a xenograft mouse tumor model.

Poster Presentation : **ORGN.P-220**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Performance improvement of Y-series based acceptors through halogenation of terminal groups

Hoeon Baek, **Yun Hi Kim**[1,*]

Chemistry, Gyeongsang National University, Korea

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

OPV demonstrates tremendous potential as an autonomous off-grid energy source for driving multiple wireless low-power IoT (Internet of Things) devices. Advances in materials have increased the power conversion efficiency (PCE) of NFA-based OPVs by about 31% compared to the beginning of the study, especially the denaturation of molecular structures with halogen groups introduced into acceptors is an effective strategy to change OPV properties. In this study, we synthesized a Y6 derivative for NFA-OPV, which introduced fluorination and chlorination. Y6 derivatives with chlorinated receptors resulted in satisfactory spectral matching, suitable energy levels, high planarity and crystallinity.

Poster Presentation : **ORGN.P-221**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthetic Studies towards Madeirolide A

Minchul Choi, Chulbom Lee[1,*]

Department of Chemistry, Seoul National University, Korea

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

Madeirolide A is a glycosylated macrolide isolated by Wright and Winder in 2009 from a marine sponge Leiodermatium species. It has been reported to possess inhibitory activity against Candida albicans, representing fungicidal MIC values of 12.51 μg/mL. Structurally, madeirolide A features three cyclic ether motifs embedded within a stereochemically decorated 24-membered macrolactone scaffold. Thus far, three partial syntheses of western fragment containing A ring of madeirolide A, including our own, have been reported. However, a complete total synthesis of madeirolide A is yet to be reported, and the absolute stereostructure and bioactivity of the natural product remains to be explored. In this poster, we present a synthetic strategy for the C13-C27 fragment of madeiorlide A. The cyclic ethers are constructed via the iridium-catalyzed visible light induced radical cyclization with high diastereoselectivity, and the assembly of the two fragments were achieved through both Michael addition and decarboxylative coupling reactions.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-222**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Calix[4]pyrrole with Extended Indole as highly selective receptor for the phosphate anion

Ju hyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new calix[4]pyrrole-based anion receptor having two diagonal amido indoles has been synthesized. It was proved by ^1H NMR spectroscopic analyses and UV/vis spectroscopic analyses that the receptor possesses an ability to recognize with high affinity oxo-anions including $H_2PO_4^-$ and $HP_2O_7^{3-}$ (as their tetrabutylammonium salts) as well as spherical halide anions in chloroform with the highest preference for the dihydrogen phosphate anion ($K_a > 10^4$). Different binding modes of the receptor for halides and the oxo-anions were revealed via ^1H NMR spectroscopic and single crystal X-ray diffraction analysis. Specifically, the receptor forms hydrogen bonds with the dihydrogen phosphate anion via the indole NHs and amide NHs as well as two pyrrolic NHs of the calix[4]pyrrole framework. In this case, the calix[4]pyrrole unit adopted the unprecedent 1,3-alternate conformation. The carbonyl oxygen atoms of the ethyl ester groups were also found to take part in the anion binding via hydrogen bond. By contrast, for halide anions, indole and pyrrolic NHs but not amide NHs took part in recognition of these anions with the calix[4]pyrrole unit locked in cone conformation.

Poster Presentation : **ORGN.P-223**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Deuterium Exchange of Pyrrolic NH Protons Accelerated by Fluoride and Bicarbonate Binding in CDCl3, CD3CN and DMSO-d6

Nam Jung Heo, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Diphenylpyrrole- and benzene-strapped calix[4]pyrroles 1 and 2 have been synthesized and their anion binding features were investigated by means of ^{1}H and ^{19}F NMR spectroscopy as well as single crystal X-ray diffraction analyses. Receptor 1 bearing an auxiliary acidic pyrrolic NH on the strap was found to bind F^- and HCO_3^- with significantly high affinity in DMSO-d_6. A combination of ^{1}H and ^{19}F NMR spectroscopic analyses revealed that fluoride binding to receptors 1 and 2 facilitates otherwise-infeasible deuterium exchanges of the pyrrole NHs from aprotic chloroform-d and acetonitrile-d_3 as well as DMSO-d_6. The bicarbonate anion was also found to bring about deuteration of the pyrrolic NHs of receptors 1 and 2 in $CDCl_3$.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-224**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Rational Design, Synthesis and Biological Evaluation of Novel Ionizable Lipid Materials for RNA Delivery

Faisal Muhammad, Soyeon Yoo[1], Gyo chang Keum[1,*], Eun-Kyoung Bang[1,*]

Organic chemistry, University of Science & Technology, Pakistan
[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

Ionizable cationic lipid-containing lipid nanoparticles (LNPs) holds great potential as an effective non-viral vector for nucleic acid-based gene therapy. This is exemplified by the two COVID-19 vaccines employing mRNA-LNP technology from Moderna and Pfizer/BioNTech. In this research work, we design and develop a chemical library of ionizable cationic lipids, and the synthesized ionizable lipids were further prepared to be LNPs using for mRNA delivery. To be more precise, the LNPs composition comprises ionized lipid, helper lipid, PEG-lipid, and additives. Through orthogonal design of experiment methodology screening, LNP-6097 containing W9MF7 shows appropriate particle size, good polydispersity index (PDI), suitable pKa, and high mRNA encapsulation efficiency. The developed W9MF7-based LNP-6097 is a promising mRNA vaccine delivery platform, and this research work delivers an overall perspective of the ionizable cationic lipids, from aspects of lipid designing, synthesis, screening, characterization, fabrication, optimization, and application.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-225**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Metal Ion Recognition of 12- and 24-Membered Macrocycle-Based Chromogenic Sensors via 1:1 and 2:2 Cyclization

Kyu Won Lee, Eunji Lee[1,*]

Gangneung-Wonju National University, Korea

[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Detection of heavy metal ions is essential because they cause serious damage to the environment and the biosystem. In this work, macrocyclic chromogenic probes with various sizes for the detection of heavy metal ion are reported. The 1:1 and 2:2 cyclization products with 12-membered and 24-membered ring cavities have been obtained from the dithiol-ditosylate coupling reaction, respectively, and successfully separated. Chromogenic sensors (L^1 and L^2) based on a NOS_2-macrocycle and $N_2O_2S_4$-macrocycle functionalized with phenyltricyanovinyl group were synthesized and characterized. L^1 can selectively detect mercury(II) ions over a series of metal ions in acetonitrile resulting in a color change of the solution from pink to pale yellow. In particular, only ClO_4^- and NO_3^- systems exhibited mercury(II) recognition, no responses were observed with other anions. The selective recognition of metal ion using the macrocyclic sensor L^2 is in progress.

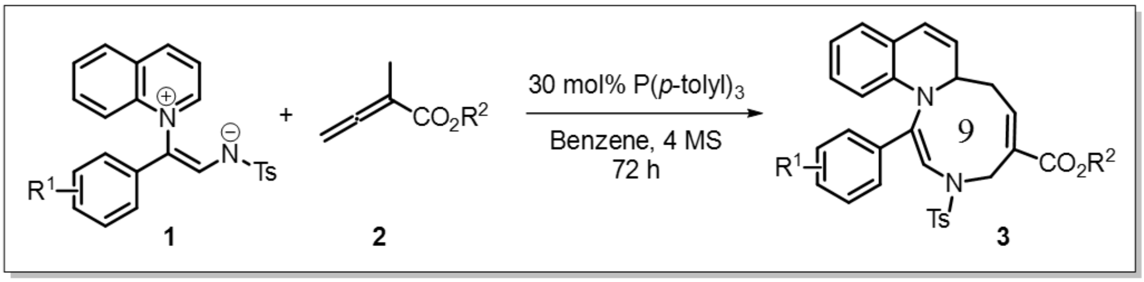
Poster Presentation : **ORGN.P-226**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Phosphine-Catalyzed [5 + 4] Cycloaddition of 2,3-Butadienoates and N-aromatic Zwitterion

Sekwang Baek, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Korea

The synthesis of nine-membered heterocycles has attracted attention due to their prevalence in natural products and biologically active compounds. There are various synthetic methods employed to create nine-membered rings, such as macrocyclization, ring expansion, and annulation. However, construction of nine-membered heterocycles presents several challenges, primarily related to entropic considerations and transannular interactions. An efficient and flexible approach is the [5 + 4] cycloaddition, involving the direct coupling of two building blocks, with one acting as a dipole and the other as a dipolarophile.In this presentation, we have disclosed a new synthesis of nine-membered N-heterocycles under mild conditions. This approach employs 2,3-butadienoates as a 1,4-dipole in the presence of a phosphine catalyst and N-aromatic zwitterion as a 5-atoms dipolarophile. In Kwon's work, a variety of tetrahydropyridine derivatives were synthesized using [4 + 2] cycloaddition via the γ-addition of allenoate and a 1,6-proton shift. In contrast, our group has developed a [5 + 4] cycloaddition utilizing a 1,9-proton shift instead of the undesired pathway through 1,6-proton shift. The application of molecular sieves allowed for the inhibition of the more easily occurring 1,6-proton shift kinetically, with further investigation underway to explain this result. The developed cycloaddition has been characterized by broad substrate scope, mild reaction conditions.


1
2
3
+
N
N
Ts
R1
CO2R2
30 mol% P(p-tolyl)3
Benzene, 4 MS
72 h
9

Poster Presentation : **ORGN.P-227**

Organic Chemistry

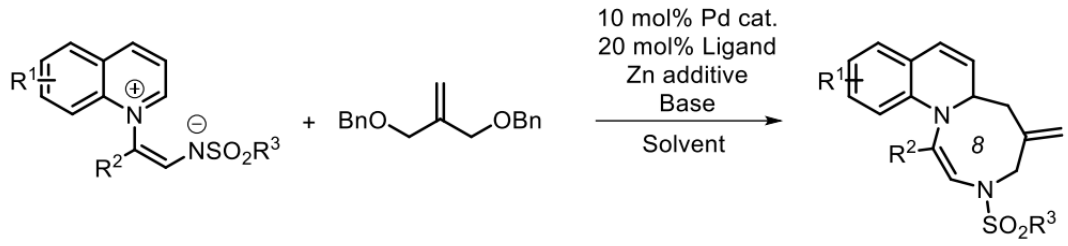
Exhibition Hall C FRI 11:00~13:00

[5 + 3] Cycloaddition of N-Aromatic Zwitterions by Switching Regioselectivity of Metal-Allyl Species

Sumin Lee, Eun Jeong Yoo*, Sekwang Baek

Department of Applied Chemistry, Kyung Hee University, Korea

Compared to synthetic approaches for typical cyclic systems, methods for constructing medium-sized cyclic compounds, especially eight-membered cyclic compounds, have been less explored due to unfavorable thermodynamics. Although eight-membered heterocyclic compounds are prevalent in natural products, biologically active molecules, and functional materials, their synthesis often requires tedious and complex stepwise reactions, rather than modular methods. Previously, we developed a new type of reactant, N-aromatic zwitterions, for the construction of medium-sized heterocyclic compounds in a modular manner. In addition, we demonstrated that N-aromatic zwitterions can undergo regiodivergent cycloadditions, depending on the nature of the reaction partners. Specifically, when the zwitterion reacts with LUMO-controlled amphiphilic reactants, it undergoes [5 + n] cycloadditions, whereas, in the presence of HOMO-controlled dipolar species, regiodivergent [m + 2] cycloadditions occur. For example, the reaction of N-aromatic zwitterions with Pd-TMM underwent a [3 + 2] cycloaddition reaction via regioselective 1,4-dearomative addition of Pd-TMM. In this symposium, we introduce a new strategy for a [5 + 3] cycloaddition of N-aromatic zwitterions and π-allyl precursors in the presence of palladium catalyst, which ensures diversity that differs from previous reports. Under the typical reaction conditions for the generation of Pd-allyl species, the additional use of zinc salt resulted in a transmetallation, affording the Zn-allyl intermediate. It readily chelated with the N-aromatic zwitterion, switching its regioselectivity which resulted in [5 + 3] cycloaddition, not [3 + 2] cycloaddition. The key intermediate was isolated and fully identified, proving the reaction mechanism involved in the formation of the Zn-allyl complex. In addition, we demonstrated the potential of this strategy for synthesizing large cyclic compounds, otherwise difficult to construct.


R1
NSO2R3
R2
+
BnO
OBn
10 mol% Pd cat.
20 mol% Ligand
Zn additive
Base
Solvent
R1
N
8
R2
N
SO2R3

Poster Presentation : **ORGN.P-228**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Structural Studies in Valine-based D/L-Peptides Introducing Cyclic β-Aamino Acids

Mireu Kim, Soo Hyuk Choi[*]

Department of Chemistry, Yonsei University, Korea

D/L-peptides are a class of molecules which can be characterized by the alternating D-amino acids and L-amino acids. These hybrid peptides with distinctive sequences can be found in nature, such as Gramicidin A, and show attractive features as a therapeutic agent. However, the high toxicity and low biocompatibility of D/L-peptides have challenged their application for the development as pharmacotherapeutic molecules. To further utilize this interesting biomolecule, studies on the biomimetic molecules that resemble the characteristic structure of D/L-peptide are essential.In this study, we designed and synthesized several peptides analogous of valine-based D/L-peptides with unnatural β-amino acid. The (1S,2R)-*cis*-2-aminocyclohexane carboxylic acid (*cis*-ACHC) was introduced into the D/L-peptide sequences to diversify the conformation of D/L-peptides. The structure of our designed peptides was investigated through circular dichroism spectra, NMR analysis, and single crystal XRD.

Poster Presentation : **ORGN.P-229**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Palladium-Catalyzed Enantioselective [3 + 2] Cycloaddition of N-Aromatic Zwitterions and Vinylcyclopropanes

Juno Im, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Korea

In the presence of a palladium catalyst, vinylcyclopropanes (VCPs) readily convert Pd-allyl cation intermediate followed by ring-opening of cyclopropanes and act as 1,3-dipoles, which have been utilized to construct five-membered cyclic compounds via 1,3-dipolar cycloaddition. This approach to generating practical 1,3-dipole has been also used to structure various molecular skeletons, such as seven-membered ring systems, multi-fused cyclic compounds, and spiro compounds. In our laboratory, cycloadditions of N-aromatic zwitterions have been developed, which provide diverse N-heterocyclic compounds whiles switching compatible reacting partners in a modular manner. For example, we have successfully developed a series of [m + 2] cycloadditions via the cycloaddition between N-aromatic zwitterions and 1,n-dipolar species bearing palladium-allyl cation moiety. In this symposium, we discuss a [3 + 2] cycloaddition of N-aromatic zwitterions and VCPs in the presence of palladium catalyst and electron-rich phosphine ligands to afford fused five-membered cyclic systems. Also, an asymmetric version of the developed cycloaddition, which gives a wild range of N-heterocycles with high enantiomeric excess, is presented. The developed methodology is significant in the field of heterocyclic synthesis because it can provide biologically active molecular skeletons with a high degree of complexity in a single operation.

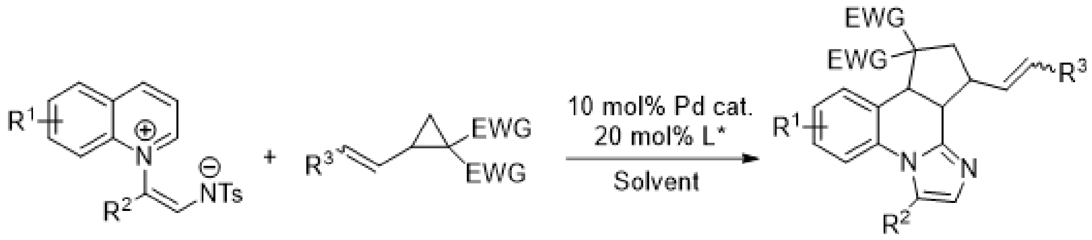


Figure 1. [3 + 2] cycloaddition of N-aromatic zwitterions and VCPs.

Poster Presentation : **ORGN.P-230**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Synergistic Activation of di-Proline-Thiouronium Salt Catalysts for Highly Enantioselective Asymmetric Michael Addition of Aldehydes to Nitroolefins

Hyoung Min Yeo, Taek Hyeon Kim[*]

School of Chemical Engineering, Chonnam National University, Korea

The symmetric Michael addition reaction offers an efficient synthetic pathway and plays a pivotal role in obtaining compounds with remarkable enantioselectivity through the reaction between aldehydes and nitroolefins. In this study, we designed di-proline-thiouronium salt catalysts with the aim of enhancing the enantioselectivity and reactivity of this reaction.By utilizing bidentate activation, interactions that are in harmony with stereochemical compatibility, and chiral recognition, their primary aim was to amplify both reactivity and enantioselectivity of these catalysts. In the experimental findings, notably higher reaction yields, pronounced syn-diastereoselectivity, and remarkable enantioselectivity were observed for both catalyst 1 and catalyst 2.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ORGN.P-231**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Conformational Analysis of α/β-Peptides and β-Peptides Containing Azepane-Derived Heterocyclic β-Amino-Acids

Ingyu Han, Chae Na Lim, Soo Hyuk Choi[1,*]

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

β-amino acids are a class of unnatural amino acids which have two carbons between the amino group and the carboxylic acid group. They are known to induce diverse structures than α-amino acids as the have an additional dihedral angle between C_α-C_β. Among them, cyclic β-amino acids are known to induce relatively stable helical structure by limiting the torsion angle between the C_α-C_β bond of the cyclic residue. However, biological application of cyclic β-amino acids still challenging as the aqueous solubility of the β-peptide is poor because of the hydrophobic cyclic residue. In this regard, introducing a heterocyclic β-amino acids instead of carbocyclic β-amino acids can be useful as heterocyclic β-amino acids can stabilize the conformation of the peptide while imposing more hydrophilicity to the backbone. In our study, we synthesized the azepane-derived (4S,5R)-5-aminoazepane-4-carboxylic acid (*cis*-AAZpC) with our simple and efficient method. Our method involved series of simple and scalable procedures like acid-catalyzed ring expansion and solvent-free reductive amination. We designed and synthesized analogues of α/β-Peptides and β-Peptides, which can display 11/9- or 12/10-mixed helices. The structure of our designed peptides was confirmed by 2D NMR analysis, circular dichroism spectra, and single crystal X-ray crystallography.

Poster Presentation : **ORGN.P-232**

Organic Chemistry

Exhibition Hall C FRI 11:00~13:00

Scalable Synthesis of *cis*-2-(Aminomethyl)cyclohexane Carboxylic Acid Using Diastereomeric Salt Formation

Heeyeon Kim, Soo Hyuk Choi[1,*]

Chemistry of department, Yonsei University, Korea

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

We synthesized the enantiomeric *cis*-2-(aminomethyl)cyclohexanecarboxylic acid with a simple and scalable method. The *cis*-2-(aminomethyl)cyclohexanecarboxylic acid is a class of γ-amino acids which asymmetric synthesis has been reported previously [1]. However, a new and improved synthetic process is necessary as the reported diastereomeric ratio between the *trans*- and the *cis*-products is about 4.8:1. In our method, we used a racemic mixture from *meso*-1,2-cyclohexanedicarboxylic anhydride as the starting material. The mixture was initially converted to a racemic mixture of the *cis*-acids. Recrystallization of diastereomeric salts with optically pure α-methylbenzylamine gave the γ-amino acid as an enantiomerically pure form, of which absolute configuration of the products was confirmed through the single-crystal X-ray diffraction analysis. This conformationally constrained cyclic γ-amino acid can be regarded as an analog of γ-aminobutyric acid (GABA) [2] and could be utilized for studying GABA-related biological mechanisms.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ORGN.P-233**
Organic Chemistry
Exhibition Hall C FRI 11:00~13:00

Nickel-Catalyzed Borylation of Aryl Fluorosulfates

Manoj Kumar Sahoo, Sung You Hong[1,*]

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

Herein, we report the nickel-catalyzed borylation of aryl fluorosulfates under mild reaction conditions. The use of near equimolar base and B_2Pin_2 loading make this method more attractive for the synthesis of various (hetero)aryl boronate esters including late-stage modification of drug molecules. Intermediate- and kinetic studies were performed to reveal the reaction mechanism.

Scheme 1. Borylation of Aryl fluorosulfates

Mechanistic and Kinetic Studies

Poster Presentation : **ORGN.P-234**

Organic Chemistry

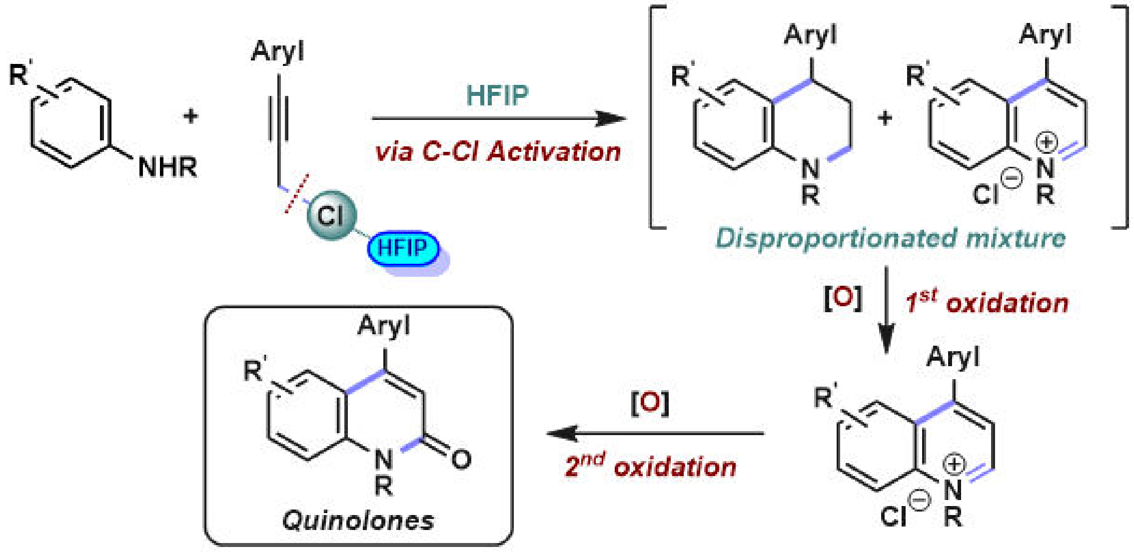
Exhibition Hall C FRI 11:00~13:00

HFIP Mediated Synthesis of C4-Arylated Quinolones via Serial Oxidation

Minseok Kang, Hyung Min Chi*

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

A practical approach for the synthesis of C4-arylated 2-quinolones from propargylic chlorides and anilines has been developed. The synthesis process involves subsequent oxidations of the initial products, tetrahydroquinolines and quinolinium ions, eventually leading to desired quinolones. A mechanism for the transformation is proposed based on a meticulous examination of intermediates and comprehensive control experiments. With a thorough understanding of the reaction mechanism, the applicability of the reaction scope is expanded.



Poster Presentation : **MEDI.P-235**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

A Cancer-Specific Cell-Penetrating Peptide BR2 for Targeted Delivery of Oxaliplatin Toward Colorectal Cancer

Jungkyun Im[*], Nasim Sepay[1], Mohuya Paul[2]

Department of Chemical Engineering, Soonchunhyang University, Korea

[1] *Department of Electronic Material and Devices Engineering, Soonchunhyang University, Korea*

[2] *Department of electronic materials, devices, and equipment engineering, Soonchunhyang University, Korea*

Oxaliplatin is extensively used in chemotherapy to treat advanced colorectal cancer (CRC), but its effectiveness is limited by poor cellular uptake and the demand for high doses, which can lead to drug resistance and adverse effects in patients. To address this issue, we attempted to utilize a cell-penetrating and cancer-specific peptide called BR2 for synthesizing a new peptide-drug conjugate. The conjugate was synthesized by conjugating oxaliplatin covalently with BR2 using a heterobifunctional linker. The resulting conjugate (BR2-Oxal) was examined for in vitro and in vivo effectiveness toward human colon cancer cells and tumors. Compared to the parent drug, in vitro investigations showed enhanced cellular uptake of BR2-Oxal with a significantly greater reduction in colon cancer cell viability leading to a higher ratio of apoptosis. In addition, we found that BR2-Oxal exhibited higher accumulation of the drug and greater tumor suppression than oxaliplatin in a xenograft mouse model, suggesting BR2-Oxal was efficiently and specifically delivered to tumors in vivo. These findings indicate that utilizing the BR2 peptide for intracellular delivery of oxaliplatin presents a promising drug delivery strategy. Also, this approach has the potential to facilitate the development of oxaliplatin prodrugs or derivatives with enhanced efficacy.

Poster Presentation : **MEDI.P-236**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Confirmation of Synergistic Anti-inflammatory and Anti-aging Efficacy of Complex Extracts from *V. rotundifolia* and *I. okamurae*

Mingyeong Kim, Dain Um[1], Shin Minyoung[2], Eun-Seok Oh[3], Sang Yun Kim[3], Chi-Young Yun[4], Byong Wook Choi[1], Bong Ho Lee[*]

Department of Chemical and Biological Engineering, Hanbat National University, Korea

[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

[2]*Chemical Biotechnology, Hanbat National University, Korea*

[3]*MSCospharm Inc., Korea*

[4]*Administration, MS Cospharm Inc., Korea*

Aligned with the trends of environmental and ethical consumption, the domestic vegan cosmetics market in South Korea has experienced an almost fourfold increase in size over the past decade. "*V. rotundifolia*", easily obtainable from the land of Jeju Island, is composed differently depending on its parts such as leaves, stems, and fruits. However, it is known to contain terpenes, flavonoids, and viterifolins, also "*I. okamurae*", a type of brown algae from the sea of Jeju Island, includes effective compounds like Diphlorethohydroxycarmalol(DPHC), 6,6'-bieckol among polyphenols, and fucoxanthin, making it valuable as a naturally-derived ingredient. In our study, we measured the anti-aging activity of a 70% ethanol extract of *V .rotundifolia* and *I. okamurae*. Particularly, when the 1:1 mixture(1 μg/mL) was treated to HMC-1 (human mast cell line), a strong synergistic effect was observed, reducing IL-4 expression by over 70%. The mixture showed no significant cell toxicity up to a concentration of 100 μg/mL. Our results suggest that the combination of *V. rotundifolia* and *I. okamurae* when used together, can serve as a more effective functional ingredient for anti-inflammatory and anti-aging purposes.

Poster Presentation : **MEDI.P-237**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of Cleavable Linker Conjugated Silica Nanoparticles for Theranostics

Myeongju Shin, Sun-Joon Min[1,*]

Applied Chemistry, Hanyang University, Korea

[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Silica nanoparticles (SNPs) are utilized as drug carriers due to their colloidal stability and large surface area. In general, surface modification of SNPs with suitable organic linkers is required to covalently introduce therapeutic or imaging materials onto SNPs with high loading efficiency. A disulfide bond, which is vulnerable to a low pH environment, can be selectively cleaved inside a tumor cell through thiol-disulfide exchange due to 100-fold high level of glutathione in tumor cells compared to that in normal cells. Thus, disulfide bond conjugated SNPs would be a thiol-responsive drug delivery platform to release a payload in a specific redox microenvironment.In this study, we described the synthesis of a traceless disulfide linker which can be incorporated on the surface of SNPs for targeted therapy. According to our previous study, this disulfide linker will also have dual functional groups, which can be conjugated with an active compound and a targeting ligand in a bioorthogonal fashion. Finally, the preliminary result of our SNPs' efficacy for cancer chemotherapy will be presented.

Poster Presentation : **MEDI.P-238**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Optimization and evaluation of pyridinyl vinyl sulfones as Nrf2 activator for the antioxidant and anti-inflammatory effects

Byungeun Kim, Ki Duk Park[1,*]

Bio-Medical Science & Technology, University of Science and Technology, Korea

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

Many studies have reported that chalcone-based compounds exhibit biological activities such as anticancer, antioxidant, anti-inflammatory and neuroprotective effects. Among the published chalcone derivatives, (E)-1-(3-methoxypyridin-2-yl)-3-(2-(trifluoromethyl)phenyl)prop-2-en-1-one (VEDA-1209), which is currently undergoing preclinical study, was selected as a starting compound for the development of new nuclear factor erythroid 2-related factor 2 (Nrf2) activators. Based on our previous knowledge, we attempted to redesign and synthesize VEDA-1209 derivatives by introducing the pyridine ring and sulfone moiety to ameliorate its Nrf2 efficacy and drug-like properties. Among the synthesized compounds, (E)-3-chloro-2-(2-((3-methoxypyridin-2-yl)sulfonyl)vinyl) pyridine (10e) was found to have approximately 16-folds higher Nrf2 activating effects than VEDA-1209 (10e: EC50 = 37.9 nM vs VEDA-1209: EC50 = 625 nM) in functional cell-based assay. In addition, 10e effectively improved drug-like properties such as CYP inhibition probability and metabolic stability. Finally, 10e demonstrated excellent antioxidant and anti-inflammatory effects in BV-2 microglial cells and significantly restored spatial memory deficits in lipopolysaccharide (LPS)-induced neuroinflammatory mouse models.

Poster Presentation : **MEDI.P-239**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Enhance skin smoothness and boost skin suppleness by fortifying adenosine's absorption into the outermost layer of the skin.

Chae Yeong Hong, Sung-Joo Hwang[1,*], Soo Ho Yeo[2,*]

Yonsei University, Korea
[1]college of pharmacy, Yonsei University, Korea
[2]Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

Adenosine constitutes one of the four nucleosides with a broad spectrum of pharmacological impacts, encompassing antineoplastic, anti-inflammatory, antioxidative, and anti-aging attributes. Its capacity to induce fibroblast growth and collagen synthesis when penetrating the skin leads to diminished skin creases and enhanced skin flexibility.To enhance the skin penetration of adenosine, which has relatively restricted permeability, we harnessed unbound fatty acids to fashion liquid nanoparticles. These nanoscale particles were employed in studies on dermal permeation carried out using rat skin.The lipid nanoparticles exhibited a particle size varying from 82.22 nm (F3) to 177.7 nm (F1).All lipid nanoparticles displayed a polydispersity index ranging from 0.19 to 0.41, indicative of a consistent and even preparation of the lipid nanoparticles.The adenosine-containing lipid nanoparticles showcased an encapsulation efficacy ranging from 55.96% to 66.79% and a drug loading content spanning 2.72% to 9.09%.Formulations demonstrated zeta potential values extending from -21.87 mV (F1) to -23.08 mV (F3).As a result, our lipid nanoparticle encapsulating adenosine presents substantial potential in boosting skin permeation and offering a prolonged anti-aging outcome.

Poster Presentation : **MEDI.P-240**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Optimizing the Preparation of Lysozyme-Loaded Liposomes through Microfluidic Process Parameter and Lipid-Cholesterol Composition Optimization

Minji Choi, Sung-Joo Hwang*

Yonsei University, Korea

Traditional methods of producing liposomes containing proteins encounter difficulties related to maintaining stability, such as protein denaturation, aggregation, agglomeration, and drug adsorption. In contrast, microfluidic technology offers distinct advantages, including precise control over particle size, consistent results, minimized reagent usage, and enhanced stability when compared to traditional methods like thin film hydration. This research aims to harness microfluidic technology for the creation of protein-loaded liposomes and optimize key parameters like the lipid (DSPC: cholesterol) molar ratio, total flow ratio (TFR), and flow rate ratio (FRR). For this study, Lysozyme, a 14 Kda protein, serves as a model drug. The ultimate goal is to identify the optimal combination of these parameters that yields the smallest particle size and the highest encapsulation efficiency for the protein drug.Based on data, the optimal formulation for microfluidics technology, achieving the highest EE% while maintaining particle size < 250 nm and PI% < 25%, was identified as F1(DSPC: cholesterol=2:1) at TFR 5 ml/min and FRR 3:1. Consequently, this formulation was selected as the most suitable for lysozyme-loaded liposomes.Through the systematic investigation of factors such as cholesterol concentration, total flow ratio (TFR), and flow rate ratio (FRR), we have achieved notable outcomes, including the reduction of liposome size, enhanced stability, and improved encapsulation efficiency. These noteworthy findings provide valuable insights into the enhancement of hydrophilic drug-loaded liposomes using microfluidics technology.

Formulation	Lipid molar ratio (DSPC : Cholesterol)	Total Flow Ratio (TFR)	Flow Rate Ratio (FRR)	Particle size (PS nm)	Polydispersity (PI %)	Zeta potential (mV)	Encapsulation efficiency (EE %)
F1	2:1	1.5	2:1	236.8±40.32	25.4±3.6	-	-
			3:1	245.8±18.61	26.5±2.1	-	-
			4:1	546.3±313.6	28.6±5.9	-	-
		3.0	2:1	179.07±5.28	25.3±1.1	-21.8±14.2	-
			3:1	192.53±15.06	27.3±0.9	-21.4±14.0	-
			4:1	357.5±104.41	25.3±0.3	-19.4±4.0	-
		5.0	2:1	134.74±1.99	23.1±1.1	-16.9±10.5	69.87±1.18
			3:1	147.53±11.08	25.5±2.0	-14.5±7.2	70.0±1.05
			4:1	137.61±1.36	26.0±0.8	-11.2±2.4	-
F2	3:2	1.5	2:1	206.7±22.37	27.5±2.3	-	
			3:1	218.0±39.48	28.8±1.0	-	-
			4:1	208.8±32.35	29.9±3.0	-	-
		3.0	2:1	148.75±10.57	25.3±2.1	3.0	-
			3:1	146.19±1.92	23.6±0.7	-5.6±2.2	-
			4:1	187.59±13.82	26.2±1.3	-5.5±6.6	-
		5.0	2:1	110.68±2.57	19.6±5.0	-4.8±0.3	34.96±0.44
			3:1	108.17±1.74	21.1±1.5	-5.5±0.7	43.07±6.94
			4:1	134.27±5.04	24.9±0.7	-5.2±3.2	50.92±14.2
F3	7:3	1.5	2:1	1296.7±150.63	36.9±6.3	-	-
			3:1	1049.8±328.2	36.4±1.6	-	-
			4:1	1577.3±939.9	33.4±4.2	-	-
		3.0	2:1	1474.4±1185.0	28.7±2.2	-	-
			3:1	462.8±69.60	26.8±2.5	-	-
			4:1	403.1±210.3	26.6±4.5	-	-
		5.0	2:1	196.04±14.40	26.0±1.7	-	-
			3:1	184.10±12.81	26.3±1.0	-	-
			4:1	219.5±30.96	26.9±2.4	-	-
F4	4:1	1.5	2:1	641.8±126.04	32.2±2.7	-	-
			3:1	1327.6±289.5	36.3±9.8	-	-
			4:1	1651.9±402.9	39.1±1.1	-	-
		3.0	2:1	730.0 ±126.54	29.9±6.8	-	-
			3:1	1003.1±269.5	28.6±7.6	-	-
			4:1	2222±1702.6	39.5±2.2	-	-
		5.0	2:1	888.1±562.9	36.6±6.0	-	-
			3:1	802.1±334.1	30.6±3.4	-	-
			4:1	940.3±357.2	30.9±4.7	-	-

Poster Presentation : **MEDI.P-241**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhancing Solubility and Efficacy of Purpurin-18-loaded Solid Lipid Nanoparticles for Photodynamic Therapy in Cancer Treatment

JooYeon Lee, Il Yoon[1,*], Sung-Joo Hwang[*], Soo Ho Yeo[2,*]

Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

[2]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*

Purpurin-18 (P18) is a crucial photosensitizer utilized in photodynamic therapy (PDT); however, its hydrophobic nature leads to facile coalescence and limited bioavailability. The objective of this research was to produce P18 through synthesis and develop P18-loaded solid lipid nanoparticles (SLNs) to enhance its bioavailability.The SLNs displayed an average particle size ranging from 164.70 to 762.53 nm, with a zeta potential ranging from -16.77 to 25.54 mV. Through the 1,3-diphenylisobenzofuran (DPBF) assay, a nonbiological evaluation, we observed an improved PDT effect of P18 when encapsulated within the SLNs. In the biological phototoxicity assay conducted on HeLa and A549 cell lines, it was interesting to note that P18-loaded SLNs demonstrated cytotoxicity under light conditions but not under dark conditionsIn summary, our findings demonstrated that P18-loaded SLNs have the potential to act as a successful passive targeting strategy for anti-cancer treatment. The formulations exhibited stable and controlled release profiles. Moreover, the PDT activity of the SLNs was found to be influenced by the specific cell type and size. Overall, our developed P18-loaded SLNs present a promising approach for utilizing PDT in anti-cancer therapy.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MEDI.P-242**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhancing Methyl pyropheophorbide-a (MPPa) Delivery and Photodynamic Therapy using Solid Lipid Nanoparticles: A Promising Approach for Anticancer Treatment

Gaeun Lee, Il Yoon[1,*], Sung-Joo Hwang[*], Soo Ho Yeo[2,*]

Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

[2]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*

Photodynamic therapy (PDT) is becoming increasingly popular as an anticancer treatment due to its non-invasive nature and minimal damage to surrounding healthy tissues, while maximizing its therapeutic effects. Methyl pyropheophorbide-a (MPPa) is a photosensitizing agent used in PDT. When activated by a specific light wavelength, MPPa generates active oxygen species that cause damage to target cells. However, the low solubility of photosensitive substances like MPPa makes drug development challenging. To tackle this issue, researchers conducted a study with the goal of enhancing MPPa's solubility and PDT effectiveness by creating MPPa-loaded solid lipid nanoparticles (SLNs).The study involved several steps, including MPPa synthesis, which was confirmed using 1H nuclear magnetic resonance (1H-NMR) spectroscopy and UV-Vis spectroscopy. The synthesized MPPa was then encapsulated within SLNs through high-temperature homogenization and ultrasonic treatment. Particle size and zeta potential were measured to evaluate the SLNs. The particle size and zeta potential ranged from 231.37 to 424.07 nm and −17.37 to −24.20 mV, respectively. The researchers also assessed MPPa's pharmacological effect using the 1,3-diphenylisobenzofuran (DPBF) assay and tested its anticancer effect against HeLa and A549 cell lines.The results showed that the MPPa-loaded SLNs effectively improved PDT efficacy and demonstrated enhanced retention effects. Additionally, UV-Vis spectrophotometer measurements confirmed improved photostability of the prepared SLNs. This study suggests that utilizing SLNs loaded

with synthesized MPPa could be beneficial in cancer treatment using PDT.References(1) S. Yeo et al., Scientific Reports, 13(1), 7391 (2023).(2) S. Yeo et al, Pharmaceutics, 14, 1064 (2022)

Poster Presentation : **MEDI.P-243**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Enhancing Cancer Treatment : Synergistic Photodynamic Therapy and Chemotherapy Using Nano-Transferosomes of Purpurin-18 Sodium salt and Doxorubicin hydrochloride

Jeonghun Ahn, Il Yoon[1,*], Soo Ho Yeo[2,*], Sung-Joo Hwang[3,*]

Yonsei Institute of Pharmaceutical Sciences, College of Pharmacy, Korea
[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*
[2]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*
[3]*Yonsei University, Korea*

Chemotherapy is a widely used cancer treatment, but there are side effects due to non-selectiv treatment. Photodynamic therapy (PDT) is gaining popularity as cancer treatment due to its non-invasive nature and minimal side effects to surrounding healthy tissues. The objective of this study was to create a combined therapeutic approach by formulating nano-transferosomes loaded with Purpurin-18 Sodium salt (P18Na) and Doxorubicin hydrochloride (DOX) through synthesis and design. This approach combines photodynamic therapy and chemotherapy to enhance the treatment efficacy.The characteristics of P18Na- and DOX-loaded nano-transferosomes were assessed including particle size, polydispersity index(PdI), zeta potential, and their pharmacological efficacy was determined using the HeLa and A549 cell lines. The characteristics of the nano-transferosomes were found to range from 98.38 to 217.50 nm and −23.63 to −41.10 mV, respectively. Furthermore, the release of P18Na and DOX from nano-transferosomes exhibited a sustained pH-responsive behavior. This pH-responsive release mechanism enhances the targeted delivery of both drugs to cancer cells and minimizes leakage in the body.These results suggest that the potential of transferosome-loaded DOX and P18Na as a synergistic therapeutic approach for cancer treatment, leveraging the benefits of chemotherapy and PDT.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-244**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Development of antimicrobial agents for treatment of Mycobacterium abscessus infection

Yuri Han, Sun-Joon Min[1,*]

Applied Chemistry, Hanyang University, Korea
[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Mycobacterium abscessus is a pathogen that induces lung infectious diseases belonging to non-tuberculous mycobacterium(NTM) family. M. abscessus poses a threat to patients suffering from chronic lung diseases such as cystic fibrosis or bronchiectasis. There is no cure for M. abscessus infection because it is resistant to most of antibiotics. Thus, it is urgent to devise innovative antibacterial agents for treatment of infectious diseases derived from M. abscessus. In our previous study, we have reported DATPT is a potential lead compound for the treatment of sepsis. Since DATPT also showed significant antimicrobial activities against several pathogenic bacteria, we have applied a chemical library of DATPT analogues to identify a hit compound through phenotypic screening against various M. abscessus strains. Among the tested compounds, OMCL18006 and 18016 showed the highest inhibitory activities against M. abscessus strains with MIC values of 5.8 μM and 4.0 μM respectively. Furthermore, the in vivo study confirmed that oral administration of OMCL18006 to the M. abscessus infected mouse model significantly reduced the population of bacteria. Currently, optimization of these active compounds to improve its potency and drug-like properties is in progress.

Poster Presentation : **MEDI.P-245**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of Phthalic Hydrazide Scaffold Tankyrase Inhibitors

Juhan Lee, Kyumyung Lee[*]

Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea

The Wnt/*β*-catenin pathway is a crucial signaling pathway involved in various cellular processes, including embryonic development, tissue regeneration, and cell proliferation. It plays a significant role in maintaining tissue homeostasis and regulating gene expression. Dysregulation of this pathway has been implicated in various diseases, including cancer. Tankyrase is an enzyme that regulates the Wnt/*β*-catenin pathway by targeting Axin, a key component of the destruction complex. Tankyrase has an ADP-ribosylase activity that leads to the poly-ADP-ribosylation of Axin. This modification disrupts the interaction between Axin and other components of the destruction complex, preventing the degradation of *β*-catenin. As a result, *β*-catenin accumulates and activates target gene expression. The inhibition of tankyrase has been explored as a potential therapeutic strategy for diseases like cancer, where aberrant Wnt/*β*-catenin signaling is often observed. By blocking tankyrase activity, the destruction complex can be stabilized which leads to reduced *β*-catenin levels and potentially inhibits the uncontrolled cell proliferation associated with certain cancers. We discovered a potent hit compound that target tankyrase protein; the structure contains phthalic hydrazide core which was identified using protein structure modeling-AI technology. Hit compound was derivatized to obtain several compounds that exhibits excellent inhibition potency against tankyrase1 and 2. Based on the result, we plan to confirm *in vivo* activity and check pharmacokinetics of the compounds.

Poster Presentation : **MEDI.P-246**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Phloroglucinol Derivatives Exert Anti-inflammatory Effects and Attenuate Cognitive Impairment in LPS-induced Mouse Model

Jushin Kim, Ki Duk Park[*]

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

Neuroinflammation is an inflammatory immune response that arises in the central nervous system. It is one of the primary causes of neurodegenerative diseases, such as Alzheimer's disease and Parkinson's disease. Phloroglucinol (PG) is a natural product contained in extract of Ecklonia cava, a marine brown algae, and is reported to be antioxidant and anti-inflammatory agent. In this study, we synthesized PG derivatives to enhance their antioxidant and anti-inflammatory activity. Among PG derivatives, KDS4156 suppressed pro-oxidative and inflammatory molecule nitric oxide (NO) production more effectively than PG. Moreover, KDS4156 dose-dependently reduced the expression of proinflammatory cytokines such as IL-6, IL-1β, TNF-α, and NO producing enzyme iNOS in lipopolysaccharide (LPS)-stimulated BV-2 microglial cells. Additionally, we confirmed that KDS4156 alleviated cognitive impairment and glial activation in mouse model of LPS-induced neuroinflammation. These findings suggest that novel PG derivative, KDS4156, is a potential treatment for neurodegenerative diseases.

Poster Presentation : **MEDI.P-247**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

An Innovative Approach for Peptide Nucleic Acid (PNA) Oligomer Synthesis: Utilizing PNA Trimer Blocks in Solid-Phase Peptide Synthesis (SPPS)

Hyewon Hwang, In seok Hong[1,*], Doyeon Kim[2]

Material Dept., Seasunbiomaterials, Korea
[1] *Department of Chemistry, Kongju National University, Korea*
[2] *chemistry department, Kongju National University, Korea*

PNA, an artificially synthesized nucleic acid with a peptide backbone structure, possesses unique characteristics such as high binding affinity and specificity for complementary DNA/RNA, as well as resistance to nucleic acid-degrading enzyme. These features make PNA applicable in various bio applications. However, during the synthesis of PNA, challenges arise from side reactions like trans-acylation and cleavage reactions, which can significantly constrain the desired PNA synthesis. Particularly, gamma-modified PNAs often face frequent synthesis failures due to inefficient coupling reactions. To address this issue, we pre-synthesized less reactive steps in solution to first assemble dimer or trimer blocks, and utilizing these blocks for SPPS synthesis resulted in enhanced crude purity and yield, enabling successful synthesis of the target PNA.

Poster Presentation : **MEDI.P-248**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Long-Wavelength Absorbing Benzimidazolo-Chlorin for Enhanced Photodynamic Therapy

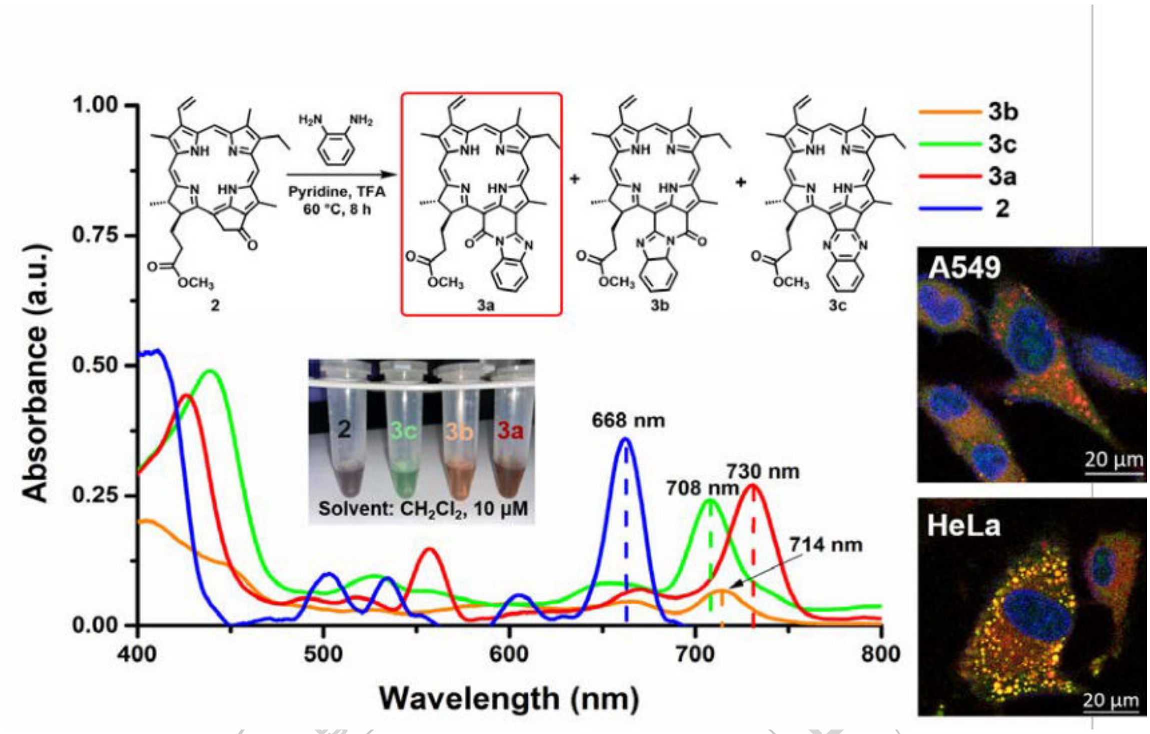
Huiqiang Wu, Soo Ho Yeo[1], Il Yoon[2,*]

Inje University, Korea

[1]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*

[2]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

The application of long-wavelength photosensitizers in photodynamic therapy has emerged as a current research focus. Due to their enhanced absorption capability in the near-infrared region and improved penetration in deep tissues, long-wavelength photosensitizers are considered as a potential strategy to enhance treatment efficacy and reduce side effects.The main content of this study was benzimidazolo-chlorin derivatives, with compound 3a used for in vitro photodynamic therapy (PDT). The results revealed that compound 3a has the potential to serve as an effective photosensitizer (PS) for enhancing PDT. Three benzimidazolo-chlorin compounds (3a, 3b, and 3c) were synthesized using methyl pyropheophorbide-a (MPPa) and 1,2-phenylenediamine. Compound 3a was characterized using UV-visible spectroscopy, nuclear magnetic resonance (1H-NMR), and high-resolution fast atom bombardment mass spectrometry. Compared to MPPa, compound 3a exhibited a significant redshift in the absorption maximum at 730 nm ($\Delta\lambda$max = 62 nm). The ability of compound 3a to generate singlet oxygen ($^1O_2$) in the near infrared range (735 nm—785 nm) and its photodynamic effects on cancer cells (A549 and HeLa) were investigated. Compound 3a demonstrated high phototoxicity, negligible dark toxicity, effective cellular uptake, and obvious aggregation in mitochondria.



1.00
0.75
0.50
0.25
0.00
Absorbance (a.u.)
400
500
600
700
800
Wavelength (nm)
H₂N NH₂
Pyridine, TFA
60 °C, 8 h
2
3a
3b
3c
3b
3c
3a
2
2 3c 3b 3a
Solvent: CH₂Cl₂, 10 µM
668 nm
708 nm
730 nm
714 nm
A549
20 µm
HeLa
20 µm

Poster Presentation : **MEDI.P-249**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Exploration of the Structure-Activity Relationship of Tirbanibulin: Synthesis and Evaluation of Amide- and Benzylamine-Modified Derivatives

Yeju Oh, Hongjun Jeon[1,*]

University of Science & Technology, Korea

[1]*Korea Research Institute of Chemical Technology, Korea*

Tirbanibulin, an FDA-approved microtubule-targeting agent in 2020, has been authorized as a pioneering therapy for precancerous actinic keratosis. The potential broadening of its application in the treatment of malignancies originates from its unique dual mechanism of action, which involves the inhibition of microtubules and Src. In this study, we presented the exploration of the structure-activity relationship of the core structure of tirbanibulin, along with the synthesis and evaluation of a series of tirbanibulin-based analogs. The results from this study revealed the importance of the pyridinyl acetamide core structure in achieving optimal cytotoxicity. Furthermore, it was observed that modifications at the para position of the benzylamine moiety were well-tolerated. Following this, a comprehensive analysis of the selected analogs was conducted through in vitro ADME and in vivo PK evaluations, confirming their mechanism of action. These findings provide valuable insights into the development of tirbanibulin derivatives as anticancer drugs.

Poster Presentation : **MEDI.P-250**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Discovery of azaindole analogs as SGK kinase inhibitors

Dagyu Kang, Mingyu Jeon, Jieun Kim, Victor Sukbong Hong*, Jinho Lee*

Department of Chemistry, Keimyung University, Korea

The serum- and glucocorticoid-regulated kinases (SGKs) are members of the AGC kinase family and consist of three isoforms: SGK1, SGK2 and SGK3. They share 80% sequence identity in the kinase domain. SGKs play important roles in the regulation of cellular signaling pathway involved in cell proliferation, stress, survival as well as transportation of nutrients and ions such as Na^+/K^+ and Ca^{2+}. Overexpression of SGK1 causes irregular cell proliferation and leads to human solid tumors. Therefore, the SGK1 is a potential target for cancer therapy.In this study, several compounds were designed and synthesized by applying various substituents to azaindole scaffolds to inhibit SGK kinase. When a substituted benzene was introduced into the azaindole, the kinase inhibitory activity was different depending on the position of the substituent at benzene. Compounds with substituents at the B position of the phenyl ring showed stronger inhibitory activity than compounds with substituents at the A position. The most active compound, with a substituent at the B position, showed an IC_{50} value of 9 nM for SGK1 and 17 nM for SGK2.

Poster Presentation : **MEDI.P-251**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synergistic Anticancer Effects of Photodynamic Therapy and Chemotherapy Using Nanostructured Lipid Carriers Loaded with Methyl pheophorbide a and Curcumin

HyeonJeong Kim, Il Yoon[1,*], Soo Ho Yeo[2,*], Sung-Joo Hwang[*]

Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

[2]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*

One of the major health problems is cancer. Various approaches have been developed to treat cancer. Among them, photodynamic therapy (PDT) is an innovative method of treating cancer using power of light. It is a method of injecting a photosensitive substance collected in a tumor into the body and activating the substance using light of a specific wavelength. In this study, researchers synthesized a photosensitizer called methyl pheophorbide a (MPa) and designed nanostructured lipid carriers (NLCs) loaded with MPa and curcumin (Cur) to combine PDT with chemotherapy for cancer treatment. The study evaluated the properties of the synthesized MPa and NLCs loaded with MPa and Cur. The particle size of the NLCs ranged from 39.08 to 459.43 nm, which is within the ideal range for better permeability and retention in cancer treatment. The pharmacological effects of MPa and Cur were tested on human cervical carcinoma (HeLa) and human lung carcinoma (A549) cell lines using NLCs in both single and combined doses. The combined administration of MPa and Cur demonstrated a stronger anticancer effect compared to the individual administrations. Therefore, the MPa- and Cur-loaded NLCs hold promise as an effective anticancer strategy by combining chemotherapy and PDT.

Poster Presentation : **MEDI.P-252**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhanced Deep-Tumor Penetration and Anticancer Efficacy of SIWV Peptide-Functionalized Porous Silicon Nanoparticles in Glioblastoma Multiforme

Eun Woo Seo, Dokyoung Kim[1,*]

Biomedical Science, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Glioblastoma multiforme (GBM) stands as a formidable challenge in oncology due to its aggressive nature and limited responsiveness to conventional chemotherapy. Addressing the constraints posed by anatomical specificity, inadequate drug targeting, and limited penetration depth, we present a novel study employing nanoparticle-based drug delivery systems (DDS) for GBM treatment. We engineered four distinct nanoparticle variants using porous silicon nanoparticles (pSiNPs) incorporating polyethylene glycol (PEG), the cancer-targeting iRGD peptide, and the newly identified GBM-targeting SIWV tetra-peptide. This research delves into their penetration capabilities within cell spheroids, GBM patient-derived tumoroids, and GBM xenograft mice models. Remarkably, our investigation reveals that the SIWV tetra-peptide exhibits a remarkable ability to enhance the penetration depth of pSiNPs. The therapeutic formulation employing SIWV-functionalized pSiNPs, loaded with the anticancer agent temozolomide, emerged as particularly efficacious, outperforming alternative formulations. These findings hold immense potential for advancing nanotherapeutics and peptide-conjugated drugs tailored for GBM treatment. As the quest for more effective therapeutic strategies against GBM persists, our study contributes vital insights for the development of innovative approaches to combat this relentless malignancy.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MEDI.P-253**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Formulation and development of rivastigmine sustained-release tablets

Hyesoo Kim, Sung-Joo Hwang*

Yonsei University, Korea

The study aims to create a sustained-release tablet form of rivastigmine tartrate, a common inhibitor for Alzheimer's and Parkinson's treatment, with the goal of minimizing gastrointestinal side effects associated with its use. The investigation focuses on utilizing hydroxypropyl methylcellulose (HPMC), Eudragit® L 100, and Lambda carrageenan as additives to develop a sustained-release matrix drug delivery system that controls drug release.The manufacturing process for the sustained-release tablets involved multiple steps using a rotary tablet press machine through direct compression. To assess the compatibility of rivastigmine tartrate with the additives (HPMC, Eudragit® L 100, and Lambda carrageenan), a melting temperature evaluation was conducted. Importantly, no significant changes were observed in the temperature peaks, indicating no substantial interactions between rivastigmine tartrate and the additives.Dissolution tests were performed to evaluate how the polymers affected the tablet's dissolution profile. Eudragit® L 100 seemed to decrease the dissolution rate due to electrostatic attraction after changing the buffer. The quantity of Lambda carrageenan also caused a notable difference in dissolution rate.The formulation of the tablets varied depending on the presence and amount of HPMC, Eudragit® L 100, and Lambda carrageenan in the mixture.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-254**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Cationic purpurinimide-polyoxometalate supramolecular complex for photodynamic and chemo combination therapy

SeungHun Kwak, Soo Ho Yeo[1], Il Yoon[2,*]

Inje University, Korea
[1]Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea
[2]Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea

Many photodynamic therapy (PDT) researchers have used polyoxometalate (POM) as a carrier for photosensitizer (PS). However, the direction of POM as a chemotherapy (chemo) to overcome two important disadvantages of PDT, low light penetration and low oxygen concentration in vivo, was not considered. This study provides the possibility of more effective PDT-chemo combination therapy using PS-POM complex as a simultaneously acting with dual role of POM as a chemo and carrier of PS, and can be widely applied to various problems.

Poster Presentation : **MEDI.P-255**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and biological study of JAK1 selective inhibitors for the treatment of autoimmune conditions

Santosh Shivanand Raikar, Pilho Kim[1,*]

Medicinal chemistry & Pharmacology, University of Science & Technology/ KRICT School, India

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

Autoimmune and inflammatory conditions are widespread and come in many forms, capable of impacting any part of the body so 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. While non-selective JAK inhibitors could lead to off-target effects and potential toxicity, selective inhibitors could offer greater specificity and reduce side effects. Filgotinib, a promising JAK1 selective 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, we designed novel compounds derived from filgotinib. Our optimization process, biological activities and ADME/Tox profiles of selected compounds will be discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-256**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Application of Lipid Nano-carrier formulation of Methyl pheophorbide-a for Enhanced Anti-cancer in Photodynamic Therapy

Soo Ho Yeo[*], Huiqiang Wu[1], Il Yoon[1], Sung-Joo Hwang[2]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

[2]*College of Pharmacy, Yonsei University, Korea*

Photodynamic therapy (PDT) is an innovative approach in cancer therapy for minimally invasive technique and selective cytotoxic effect, unlike chemotherapy. Methyl pheophorbide-a (MPa) is one of the photosensitizers (PSs) that are essential active pharmaceutical ingredients (APIs) in PDT. The reactive oxygen species (ROSs) generated from PS lead to cancer cell apoptosis after irradiating the light. Lipid nano-carrier formulation is one of the drug delivery systems for enhanced bioavailability of API in pharmaceutics. Particularly, its induces cellular uptake of API due to its lipophilic property. Therefore, we represent that synthesized MPa and MPa loaded lipid nano-carrier formulation.

Poster Presentation : **MEDI.P-257**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Design and Synthesis of Large Tumor Suppressor Kinase 1/2 Inhibitors with the Core Scaffold of 2-(Pyridin-4-yl)quinazoline

Hongjun Jeon*, Minji Kang

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

The Hippo signaling pathway is a regulatory pathway that governs organ size in animals by controlling cell proliferation and apoptosis. At the core of the Hippo pathway, Large Tumor Suppressor Kinase 1/2 (LATS1/2) plays a pivotal role as a central mediator. LATS1/2 is responsible for phosphorylating YAP and TAZ proteins, triggering their cytoplasmic sequestration and degradation. When LATS1/2 is inactivated, unphosphorylated YAP/TAZ molecules translocate to the nucleus and initiate the transcription of genes associated with cell proliferation. Recent research reveals that this nuclear translocation of YAP/TAZ induces the transcription of Vestigial-Like Protein 3 (VGLL3), subsequently recruiting the NCOR2/SMRT repressor complex to the super-enhancer region of the ESR1 gene. Therefore, a small molecule inhibitor targeting LATS1/2 can function as a repressor for the ESR1 gene, offering potential application in ER-positive breast cancer patients, even with ESR1 gene mutation. Here, we present the design and synthesis of a LATS1/2 inhibitor featuring a 2-(pyridin-4-yl)quinazoline core, derived from the known LATS1/2 inhibitor VT-02956. The primary objectives of this medicinal chemistry program are: 1) to retain or enhance the LATS inhibitory efficacy compared to that of VT-02956, and 2) to improve the metabolic stability of VT-02956.

Poster Presentation : **MEDI.P-258**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Encapsulation of Methyl pheophorbide-a in Nano-transfersomes for pH-responsive drug delivery system in Photodynamic Cancer Therapy

Soo Ho Yeo*, Huiqiang Wu[1], Il Yoon[1], Sung-Joo Hwang[2]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

[2]*College of Pharmacy, Yonsei University, Korea*

Methyl pheophorbide-a (MPa) is an essential photosensitizer (PS) in photodynamic therapy (PDT). PDT is a light-based cancer treatment, which is advantageous to overcome non-specific cancer therapy as chemotherapy. Despite its non-invasive and patient-friendly cancer therapy, many PSs have lipophilic property, which causes poor bioavailability. Transfersome is pH-responsive pharmaceutical formulations with ampiphilic property. The nano- technology is one of the passive targeting strategy using the enhanced permeability and retention (EPR) effect in cancer therapy. Thus, we exhibit that synthesized MPa and nano-transfersomes for pH-responsive drug delivery system.

Poster Presentation : **MEDI.P-259**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Lipid Nanoparticle of Curcumin for Advanced Chemotherapy of Cancer

Soo Ho Yeo[*], **Huiqiang Wu**[1], **Young Key Shim**[2], **Il Yoon**[1], **Sung-Joo Hwang**[3]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea
[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*
[2]*Department of Nano Convergence Engineering, Inje University, Korea*
[3]*College of Pharmacy, Yonsei University, Korea*

Curcumin (Cur) Cur is a yellow phytochemical substance approved as a safe compound by the World Health Organization and US Food and Drug Administration (FDA). Various preclinical studies over the last two decades have shown that Cur possesses potent anticancer property. Cur is known as the biopharmaceutical classification system (BCS) class 4 drug that is low solubility and permeability. Lipid nanoparticle (LN) is advantageous formulation for delivering BCS class 4 drug owing to its lipid nature. In LN system, a lipophilic drug is stably dispersed in the water solvent via encapsulation into the lipid matrix. Herein, we exhibit our Cur-encapsulated LN formulation for advanced cancer chemotherapy. Three cell lines (HeLa, A549, and CT-26) were assessed

Poster Presentation : **MEDI.P-260**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Design of Solid Lipid Nanoparticles to Improve Skin Barrier Permeation of Adenosine

Soo Ho Yeo*, **Sung-Joo Hwang**[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Skin is the largest organ in the body and covers the body's entire external surface. It consists of three layers, which are the epidermis, dermis, and the hypodermis. The epidermis is the outermost layer made up of keratinocytes that secrete keratin protein, intercellular lipids to form the ECM, melanocytes to produce pigment, and Langerhans cells to present antigen. The epidermis layer acts as a skin barrier to protect the internal organs from environmental toxins. Adenosine, an active cosmeceutical ingredient, has hydrophilic property that is one of the limitation for permeation of skin barrier. Solid lipid nanoparticle (SLN) is advantageous for cosmeceutical formulation owing to using biocompatible lipid and affinity with intercellular lipids. The aim of this study is to fabricate adenosine-encapsulated SLN for improved skin permeation. Regarding biological examination, according to the EU Cosmetics Directive prescribed the use of alternative methods to animal testing.

Poster Presentation : **MEDI.P-261**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Lipid Nanocarrier-incorporated Elastic Artificial Skin Formulation for Topical Delivery of Adenosine

Soo Ho Yeo*, **Sung-Joo Hwang**[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Adenosine (AD) is one of an active cosmeceutical ingredient approved for the treatment of anti-winkle effects. AD chemically induces the synthesis of collagen in fibroblasts. AD is difficult in penetrating the skin due to its hydrophilicity. Lipid nanocarrier (LN) is an effective formulation to improve skin penetration for hydrophilic drugs. Its lipophilic property assists close interaction of lipid nanocarrier with skin. Elastic artificial skin formulation physically pulls the applied skin with adhesive force. Elastic artificial skin is a highly convenient topical drug delivery system owing to its rapid formation via a cross-linking reaction. In this report, we fabricated AD-encapsulated LN incorporated into elastic artificial skin for improved anti-winkle using both chemical and physical mechanism.

Poster Presentation : **MEDI.P-262**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Phospholipid-based Solid Dispersion Formulation of Aprepitant for Enhanced Bioavailability

Soo Ho Yeo[*], **Sung-Joo Hwang**[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Aprepitant (APR) is a Biopharmaceutics Classification System class II (BCS class II) drug. Its low solubility property induces the rate-limiting step for their gastrointestinal absorption. Solid dispersion (SD) formulation has been used for BCS class 2 drugs.to enhance the solubility and dissolution rate. Traditionally, SD uses the hydrophilic polymer ingredients, which is a concern for the storage stability due to absorption of atmospheric moisture. We applied phospholipid to the ingredient of SD matrix owing to its amphiphilic property. The characteristics of chemical interaction and structure were confirmed. The solubility and dissolution rate were evaluated. Therefore, our phospholipid-based SD formulation is a promising for enhanced bioavailability.

Poster Presentation : **MEDI.P-263**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Improved Skin Moisturization Designed by Combined Formulation of Lipid Nanoparticles of Serine with Reed Root Extract

Soo Ho Yeo*, **Sung-Joo Hwang**[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Serine (Ser) is the most major component of natural moisturizing factors (NMF) that has been known to contribute to keeping the hydration state of the skin surface. However, Ser has difficult to incorporation into the stratum corneum (SC). Lipid nanoparticles (LNs) can facilitate the incorporation of Ser to the SC due to its lipophilic property. The polysaccharide-rich reed (Phragmites communis) root extract (RRE) has the hygroscopic nature leading to a considerable humectant effect. We applied RRE to hydrogel system for topical delivery of skin moisturization. Thus, we fabricated Ser as a NMF encapsulated into LN formulation, followed by combination with RRE-based hydrogel. A variety of lipid were tested to sort appropriate lipid.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-264**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

pH-sensitive Nano-transfersome of 5-fluorouracil Incorporated in Pectin-based Hydrogel for Intraperitoneal Injection

Soo Ho Yeo*, Chae Yeong Hong[1], JooYeon Lee[1], Sung-Joo Hwang[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1] *College of Pharmacy, Yonsei University, Korea*

Cancer is a devastating disease that is caused by uncontrollable growth of cells triggered from a series of genome mutations and their subsequent spread across the body. 5-fluorouracil (5FU) is one of the most frequently used cancer chemotherapy drugs. Despite its worthy cancer therapy, the utilization of 5FU still has concerns on low absorption into body, side effects, and suffering the significant hepatic first pass metabolism. Transfersome system, a liposome class carrier system, is a biocompatible lipid-based and pH-responsive carrier, which has been widely used for cancer treatment. Hydrogels are a class of three-dimensional (3D) cross-linked polymeric structures. Pectin is a substance derived from plant cell walls with mucoadhesive polymer, which induces local drug delivery after administration of 5FU. Therefore, we prepared nano-transfersome of 5FU incorporated in pectin-based hydrogel for smart cancer treatment by intraperitoneal injection.

Poster Presentation : **MEDI.P-265**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Poly(lactic-co-glycolic acid) of 5-fluorouracil Contained in Hyaluronic acid-based Hydrogel for Intraperitoneal Injection

Soo Ho Yeo*, Chae Yeong Hong[1], JooYeon Lee[1], Sung-Joo Hwang[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Cancer is one of the greatest health concerns worldwide. Colorectal malignancy is the most generally happening tumors. Various therapeutic strategies for cancer, such as surgery, radiotherapy, and chemotherapy, which can be used either alone or in combination with each other, are available. Chemotherapy, a commonly used anti-cancer strategy, has been developed by screening for natural or synthetic anti-cancer compounds. 5-fluorouracil (5FU) is one of the most frequently used among chemotherapy drugs due to its hydrophilicity. However, 5FU still has concerns on side effects and suffering the significant hepatic first pass metabolism. Poly(lactic-co-glycolic acid) (PLGA) is Food and Drug Administration approved for many formulations. The utilization of PLGA is worthy in terms of biodegradable and biocompatible ingredient. In intraperitoneal injection, residence is important for body absorption. In this regard, hydrogel formulation is advantageous for adhesion. Hyaluronic acid (HA) is known as mucoadhesive polymer. Therefore, we designed HA-based hydrogel with PLGA of 5FU formulation.

Poster Presentation : **MEDI.P-266**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Carbopol and Chitosan-based Hydrogel with Nanostructured Lipid Carriers of 5-Fluorouracil for Cancer Therapy with Intraperitoneal Injection

Soo Ho Yeo[*], **Chae Yeong Hong**[1], **JooYeon Lee**[1], **Sung-Joo Hwang**[1]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*College of Pharmacy, Yonsei University, Korea*

Colorectal cancer is the second highest diagnosed cancer in the word. The present treatment of colorectal cancer largely depends on radiotherapy, surgery, targeted therapy and chemotherapy. 5-fluorouracil (5FU) is one of the most frequently used among chemotherapy drugs due to its hydrophilicity. However, 5FU still has concerns on side effects and suffering the significant hepatic first pass metabolism. Nanostructured lipid carriers (NLCs) appear to be a promising drug delivery system for increasing stability for entrapped drugs and avoiding hepatic first pass metabolism. Especially, NLC system effectively absorbs into body due to its lipophilic property. In intraperitoneal injection, residence is important for body absorption. In this sense, hydrogel formulation is beneficial for residence for a longer period of time. When carbopol and chitosan polymeric solutions are combined, the hydrogel strength in the physiological condition could be significantly enhanced. Herein, we reported our carbopol and chitosan-based hydrogel with 5FU-entrapped NLC for intraperitoneal injection to treat cancer.

Poster Presentation : **MEDI.P-267**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

High throughput virtual screening strategy to discover novel inhibitors for E3 ubiquitin-protein ligase CBL-B with docking and machine learning

Soo Won Lee

College of pharmacy Seoul National University, Korea

In this research, we adopted a high-throughput virtual screening (HTVS) strategy, integrating docking and machine learning techniques, to find novel inhibitor candidates for E3 ubiquitin-protein ligase CBL-B. We focused on identifying candidates that are both innovative and swiftly verifiable experimentally, leading to the identification of 150 hit candidates from 3 million molecules within the Enamine REAL database. To reflect drug-likeness, we applied PAINS filters, and by confirming ordering availability, we prepared 150 final candidates for immediate synthesis and further experimental verification. Our approach underscores the potential of in silico techniques in modern drug discovery, marking a significant advancement in the field.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MEDI.P-268**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

New fibroblast activation protein (FAP)-targeted molecules based on the stilbene scaffold.

<u>Dabin Kim</u>, Ji Young Choi[1], Ho Rim Oh[2], Giuseppe Felice Mangiatordi[3], Nunzio Denora[4], Hyewon Youn[2], Hyung-Jun Im[5,*], Byung Chul Lee[1,*]

Department of Molecular Medicine and Biopharmaceutical Sciences, Seoul National University, Korea
[1]*Department of Nuclear Medicine, Seoul National University Bundang Hospital, Korea*
[2]*Department of Nuclear Medicine, Seoul National University College of Medicine, Korea*
[3]*Institute of Crystallography, National Research Council, Italy*
[4]*Department of Pharmacy – Drug Sciences, University of Bari "A. Moro", Italy*
[5]*Graduate School of Convergence Science and Technology, Seoul National University, Korea*

Da Bin Kim, Ji Young Choi, Ho Rim Oh, Giuseppe Felice Mangiatordi, Nunzio Denora, Hyewon Youn, Hyung-Jun Im, Byung Chul Lee.Cancer-associated fibroblasts (CAFs) play important roles in tumor progression and metastasis by remodeling the extracellular matrix and promoting angiogenesis. Fibroblast activation protein (FAP) is one of the most prevalent markers for CAFs and overexpressed in more than 90% of epithelial carcinomas. Additionally, its minimal expression in normal tissues positions FAP as a promising biomarker for cancer theranostics. The reported FAP inhibitors (FAPI) possess a quinoline pharmacophore that binds strongly to FAP enzyme, potentially blocking its active site or causing conformational changes that hinders its protease activity. We hypothesized that modification of quinoline moiety in FAPI could enhance the binding affinity to FAP. Instead of a quinoline moiety, six different aryl molecules were introduced to the FAPI for the in silico molecular docking simulation study using Glide. FAPI-D containing stilbene moiety exhibited the lowest binding energy (e.g. highest binding affinity) at -81.72 kcal/mol and was selected as a lead compound. Subsequently, we synthesized a fluorescent probe, Cy5.5-StGP, based on the FAPI-D, and evaluated its FAP-targeting potential in CCl_4-induced liver fibrosis mouse models. Both in vivo and ex vivo biodistribution studies showed the

remarkable uptake in the fibrotic liver selectively that has FAP overexpression compared to other organs. In addition, the result indicated not only a significant uptake of Cy5.5-StGP, but rapid clearance from the main healthy organs within just 1 hour post-injection. We anticipate that our newly developed StGP holds promising potential as FAP-targeted molecules for FAP-related diseases.

Poster Presentation : **MEDI.P-269**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Molecular Docking Analysis of 2-Phenylbenzimidazole Derivatives for the Discovery of novel mPGES-1 Inhibitors

Jayeon Lee, Minji Kim, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

Prostaglandin E_2 (PGE_2) is a key lipid mediator of inflammation. Nonsteroidal anti-inflammatory drugs (NSAIDs) and cyclooxygenase-2 (COX-2) inhibitors confer a gastrointestinal (GI) side effect and increase cardiovascular adverse events, respectively. Therefore, microsomal prostaglandin E synthase-1 (mPGES-1), a terminal synthase of PGE_2 production, has been recognized as a key enzyme in inflammatory diseases such as arthritis, atherosclerosis, stroke and cancer. This study aims to develop a novel anti-inflammatory drug as a selective mPGES-1 inhibitor. For this goal, we designed and synthesized a series of new 2-phenylbenzimidazole derivatives as a key privileged scaffold. Among them, compound MPO-0257 showed the most potent inhibitory activity against PGE_2 production (IC_{50} = 0.19 μM in A549 cells) through selective mPGES-1 inhibition (IC_{50}= 3.54 μM in a cell-free assay). Molecular docking suggests that compound MPO-0257 would inhibit PGE_2 production by blocking the PGH_2 binding site of human mPGES-1 enzyme.

Poster Presentation : **MEDI.P-270**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Biological Evaluation of Benzoxazole Derivatives for the Discovery of Novel NDRIs Antidepressants

Choi Kim, Hyemin Choi, Minju Gwon, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

Norepinephrine-dopamine reuptake inhibitors (NDRIs), the third-generation antidepressants, inhibit the reuptake of dopamine and norepinephrine. When the amount of norepinephrine increases between synapses, however, it binds to the α_2c receptor and thus a negative feedback occurs to regulate the amount of norepinephrine. To solve this problem, we decided to develop a multi-action compound that can play a role as both a norepinephrine-dopamine reuptake inhibitor and an antagonist of the α_2c receptor. Based on fragment-based drug design, a series of new benzoxazole derivatives was designed, synthesized, and biologically evaluated for the biological activity. Among them, compound 8d demonstrated excellent biological activity against α_2c receptor (binding affinity, K_i = 51.74 nM). In addition, a GluA1 phosphate experiment was conducted to confirm whether compound 8d could exhibit antidepressant effect. As a result, compound 8d was found to increase the phosphorylation of the α-amino-3-hydroxy-5-methyl-4-isoxazole propionic acid (AMPA) receptor subunit GluA1, which means that compound 8d could be a potential candidate for the discovery of novel antidepressant agent.

Poster Presentation : **MEDI.P-271**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Advancing Cancer Treatment: Pyropheophorbide-a (PPa) PPa-loaded Nanostructured Lipid Carriers

Yuim Jeon, Il Yoon[1,*], Soo Ho Yeo[*], Sung-Joo Hwang[*]

Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

Cancer is a major health threat with uncontrolled cell growth and spread. Photodynamic therapy (PDT) has emerged as a promising alternative treatment. PDT uses a photosensitizer (PS) that reacts with specific light to generate reactive oxygen species, selectively killing tumor cells without harming healthy cells. Pyropheophorbide-a (PPa) is a chlorin class PS with a long absorption wavelength but limited bioavailability. To improve PS delivery, nanostructured lipid carriers (NLCs) were developed as lipid-based Drug Delivery System (DDS) with advantages like low toxicity and high storage stability. In this study, PPa was synthesized, loaded into NLCs, and evaluated for cancer treatment using PDT. The PPa-loaded NLCs showed favorable particle characteristics. In vitro studies demonstrated the photo-cytotoxicity of the prepared PDT systems on HeLa and A549 cancer cell lines. In this study, we synthesized PPa and developed PPa-loaded NLCs for innovative cancer treatment using PDT. PPa-loaded NLCs exhibited smaller particle size, improved stability, and higher drug loading capacity compared to SLNs. They also showed superior photocytotoxicity, potentially due to enhanced cellular uptake via the EPR effect. Our PPa-loaded NLC system holds great promise as a PDT-based cancer treatment strategy.

Poster Presentation : **MEDI.P-272**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of 7-dimethylamino-6-demethyl-6-deoxytetracycline (minocycline)

Heung Mo Kang[*], **Jae Yeol Lee**[*]

Department of Chemistry, Kyung Hee University, Korea

Minocycline is a second-generation tetracycline antibiotic produced from first-generation DMCT(Dimethylchlorotetracycline). In addition, Minocycline is an essential intermediate for manufacturing third-generation tetracycline drugs (Tigecycline, Omadacycline, and Sarecycline), and commercial bulk production of Minocycline is very important.In this study, a manufacturing method for the commercial production of Minocycline is described.

Poster Presentation : **MEDI.P-273**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Utilization of PLGA Nanoparticles as Methyl pheophorbide-a Delivery Systems for Photodynamic Cancer Treatment

Heejae Choi, Il Yoon[1,*], Soo Ho Yeo[*], Sung-Joo Hwang[*]

Yonsei Institute of Pharmaceutical Sciences, College of Pharmacy, Yonsei University, Korea

[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

In this study, Photodynamic Therapy (PDT) is adopted as a method for cancer treatment, and the design of a drug delivery system using PLGA Nanoparticles (PLGA-NP) for this purpose is aimed. PDT is an innovative anti-cancer therapy that utilizes specific wavelengths and photosensitizers responsive to this light to generate reactive oxygen species, effectively eliminating cancer cells. The objective of the research is to synthesize a PDT photosensitizer, methyl pheophorbide-a (MPa), from chlorophyll, and to load it into PLGA-NP to enhance its activity. MPa faces a challenge of low bioavailability due to its poor water solubility. Therefore, a system for delivering MPa into the body is necessary to increase its bioavailability. PLGA is a synthetically derived biodegradable polymer approved by the FDA, known for its ability to undergo hydrolysis in the body. Utilizing PLGA to deliver MPa into the body not only enhances its bioavailability but also minimizes potential toxicity. As a result, successful synthesis of MPa and the design of MPa-loaded PLGA-NP led to improved PDT effects. This highlights the promising potential of the developed MPa-loaded PLGA-NP as a candidate for cancer therapy using PDT.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-274**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of mitochondria-targeted TIPTP derivatives as therapeutic agents for colitis

Siwoo Kim, Sun-Joon Min[1,*]

Applied chemistry, Hanyang University, Korea

[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Mitochondria are membrane-bound organelles that are essential for maintaining energy through oxidative phosphorylation and other metabolic functions. Reactive oxygen species (ROS) in mitochondria regulates inflammatory signaling, but ROS overproduction can lead to oxidative damage of cellular components, resulting in mitochondrial dysfunction. In our previous study, we demonstrated that the interaction between Rubicon and p22phox, increases cellular ROS level. Furthermore, an N-terminal eight amino acid (N8) peptide derived from p22phox and mimetic of N8, known as 2-(tetrahydroindazolyl)phenoxy-N-(thiadiazolyl) propenamide (TIPTP), exhibits potent anti-inflammatory effects by interrupting the interaction of Rubicon and p22phox. However, the correlation between mitochondrial ROS (mtROS) and Rubicon is not well understood. In this study, we designed and synthesized TIPTP derivatives (Mito-TIPTP), which deliver TIPTP to mitochondria selectively. They effectively inhibited the interaction of p22phox-Rubicon in mitochondria and exhibited a significant therapeutic effect in DSS-induced acute or chronic colitis mouse models by decreasing mtROS and cytokine production. Therefore, we suggest that Mito-TIPTPs would be potential therapeutic agents for treatment of intestinal inflammation.

Poster Presentation : **MEDI.P-275**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Antiviral Activity of *β*-D-*N*⁴-Hydroxycytidine (NHC) Prodrugs against SARS-CoV-2 *in vitro*

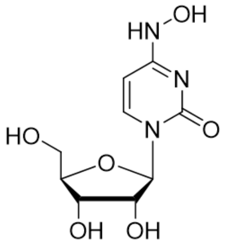
Yeon Jin An, Jong Hyun Cho[1,*], Se Myeong Choi[2], Eun Rang Choi[2], Ji Yeon Yang, Yong Hun Choi, A Young Jung[2], So Jung Kwon[2]

college of Health science, Dong-A University, Korea

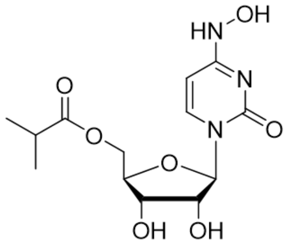
[1]*Department of Medicinal Biotechnology, College of Health Science, Korea*

[2]*Health science, Dong-A University, Korea*

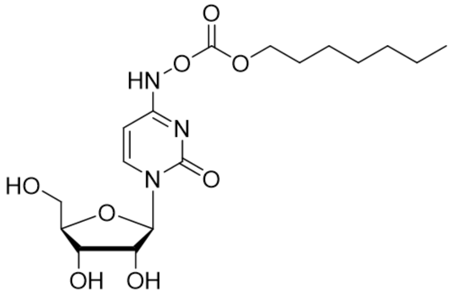
As the viral genomic mutant nucleoside agent, *β*-D-*N*^{4}-Hydroxycytidine (NHC, EIDD-1931) analogs have shown a broad spectrum of antiviral activity against RNA viruses such as SARS-CoV, MERS-CoV, norovirus, chikungunya virus, WNV, JEV, and Zika virus. Among them, MK-4482 (EIDD-2801) was developed to be a potent Anti-SARS-CoV-2 agent that causes viral RNA mutations. With the core NHC scaffold, we desinged and synthesized novel NHC analogs as prodrug forms to find a potent candidate of anti-COVID-19 treatment. In this study, we present the synthetic methods and antiviral activity of several NHC analogs modified NHC parent molecule as well as MK-4482 (EIDD-2801, treatment for SARS-CoV-2 infection). In addition, the NHC prodrugs showed potent antiviral activity (EC_{50} 1.20 μM) against SARS-CoV-2 in vitro. Especially, compound (CD-I-100) exhibited the most potency of SARS-CoV-2 (EC_{50} 1.20 μM) without cell toxicity.



NHC(EIDD-1931)



MK-4482(EIDD-2801)



CD-I-100

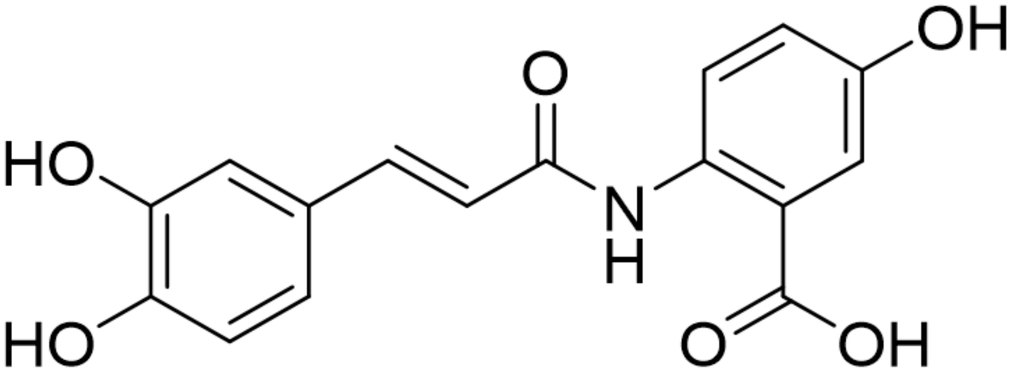
Poster Presentation : **MEDI.P-276**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Development of Practical Synthesis of Avenanthramide C Using Crystallization

So Jung Kwon, Se Myeong Choi, Yong Hun Choi, A Young Jung, Ji Yeon Yang, Jong Hyun Cho[1,*]

college of Health science, Dong-A University, Korea
[1] *Dong-A University, Korea*

Avenanthramide C (Avn C) has been known as the most potent metabolites of oats, and currently showed a variety of biological effects including Alzheimer's disease, noise-induced hearing loss, drug-induced hearing loss, and chemotherapy induced peripheral neuropathies (CIPN), etc. Unfortunately, the convenient and efficient synthesis method of Avn C has not reported in the multi-gram scale to date forwards preclinical or clinical studies. As the results, subsequent studies have been difficult to undertake despite of the promising biological activities of Avn C. In this study, we present a novel synthetic method of Avn C with convenient crystallization, or salting out instead of expensive resins to overcome the current synthetic limitations. Our method provided that the overall yield of Avn C from cinnamic acid was 70-80% in multi-gram scale with > 99.9% purity (HPLC).



Avenanthramide C

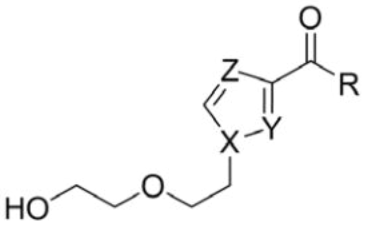
Poster Presentation : **MEDI.P-277**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Synthesis of Five-membered Hetero Cyclic Base Nucleoside Analogs and their Antiviral Activity

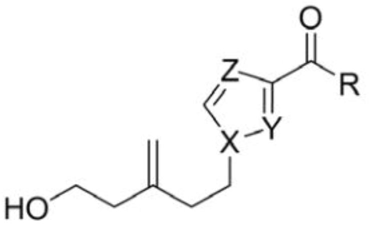
Eun Rang Choi, Eun Woo Seo[1], Yong Hun Choi[2], A Young Jung[3], Ji Yeon Yang[2], Se Myeong Choi, Yeon Jin An, So Jung Kwon, Jong Hyun Cho[*]

Dong-A University, Korea
[1]*Kyung Hee University, Korea*
[2]*college of Health science, Dong-A University, Korea*
[3]*Health science, Dong-A University, Korea*

Novel acyclic five-membered base nucleosides as the combinational structure of ribavirin and acyclovir or Entecavir were designed to find new hit compounds against RNA virus. As depicture in Fig 1, acyclic nucleosides (1a-2l) were synthesized by using Mitsunobu reaction. Mitsunobu reaction of some acyclic sugar moieties with pyrazole, imidazole, and triazole, followed by removal of protecting group(s) provided their corresponding nucleoside ester derivatives in moderate to good yield. The nucleoside esters were treated with ammonia to afford the corresponding nucleoside analogs in good yield. Additionally, the nucleoside esters were treated with methylamine to afford the corresponding nucleoside analogs in good yield. The prepared nucleosides are under investigation of antiviral activity against RNA viruses including Dengue, Flu A and SARS-CoV-2 viruses.



1a-l



2a-l

R = OMe, NH_2, $NHCH_3$

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MEDI.P-278**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Development of nano drug-delivery system for photodynamic therapy using hydrophilic and biocompatible photosensitizer-polyethyleneimine conjugate

Taemin Kim, Soo Ho Yeo[1], Il Yoon*

Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea
[1]*Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea*

Polyethyleneimine (PEI) is a polymer with repeating units consisting of an amine group and two-carbon aliphatic CH_2 CH_2 spacer. Linear PEIs contain all secondary amines, unlike branched PEIs, which contain primary, secondary and tertiary amino groups. At first, PEI has an advantage that it is a well-known biocompatible polymer with low toxicity. The reason for using PEI is that since the photosensitizer (PS) itself is hydrophobic and not water-soluble to make a low therapeutic effect in photodynamic therapy (PDT). Therefore, we combined PEI and PS to generate hydrophilic and biocompatible PS-PEI conjugate to enhance therapeutic activity in PDT based on the increased circulation time in the blood. In this poster, we will show current progress of the hydrophilic and biocompatible PS-PEI conjugate as a suitable drug-delivery system to enhance PDT activity.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-279**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

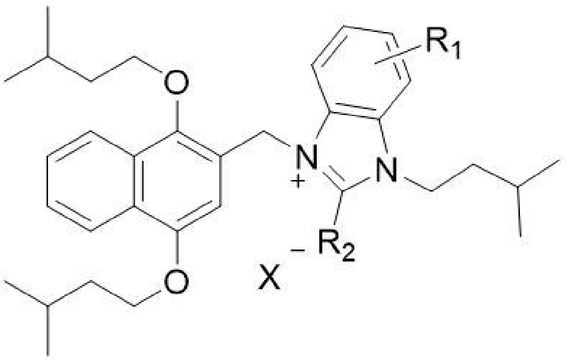
Synthesis and antitumor activity of novel 1,4-dialkoxynaphthalene-2-methyl imidazolium salts

Haena Lee, Hakwon Kim[1,*]

Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Extracellular signal-regulated kinase 5 (ERK5), a member of the mitogen-activated protein kinase (MAPK) family, is involved in key cellular processes. However, overexpression and upregulation of ERK5 have been reported in various cancers. Therefore, inhibiting ERK5 exhibits the effect of suppressing the harmful properties of cancer cells, so ERK5 has become a new target for anticancer drug development.In this study, a novel structure of 1,4-dialkoxy-2-methyl benzimidazolium salt was designed and synthesized to potentially serve as an ERK5 inhibitor. To confirm the effectiveness of these derivatives in inhibiting ERK5, their binding affinities for ERK5 were predicted using in silico analysis. The obtained results were then compared with the results of PCNA inhibition experiments.



1,4-dialkoxynaphthalen-2-methyl benzimidazolium salts

Poster Presentation : **MEDI.P-280**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Dual-targeted, NIR(near-infrared) Fluorescence-based Tumor Imaging and Therapy

Hyemi Jo, Seongyun Choi[1], Jiyoung Hyun[2,*]

Chemistry, Yonsei University, Korea

[1]*medicinal chemistry, University of Science & Technology, Korea*

[2]*data convergence drug research center, Korea Research Institute of Chemical Technology, Korea*

NIR fluorophores differ from shorter-wavelength dyes due to their longer wavelength characteristics. These fluorophores emit low-energy NIR photons that can penetrate deep into tissues with minimal damage to biological samples. They have potential as photodynamic and photothermal therapeutic agents. However, improving selectivity for cancer cells remains a focus, with ongoing research aiming to enhance specificity. Cancer cells grow rapidly due to active metabolism, often marked by an excess of β-galactosidases that process β-galactose. Glutathione(GSH), found in most cells, serves roles like detoxification, antioxidation. While GSH maintains balance in normal cells, it boosts resistance to oxidative stress in cancer cells, aiding survival, progression, and metastasis. Based on the high level of β-galactosidases and GSH in cancer cells, a new cancer theranostic reagent was developed. This utilizes a Dual-targeted NIR probe cleaved by both GSH and β-galactosidases, with potential applications in photodynamic therapy(PDT) and photothermal therapeutic agents(PTT).

Poster Presentation : **MEDI.P-281**

Medicinal Chemistry

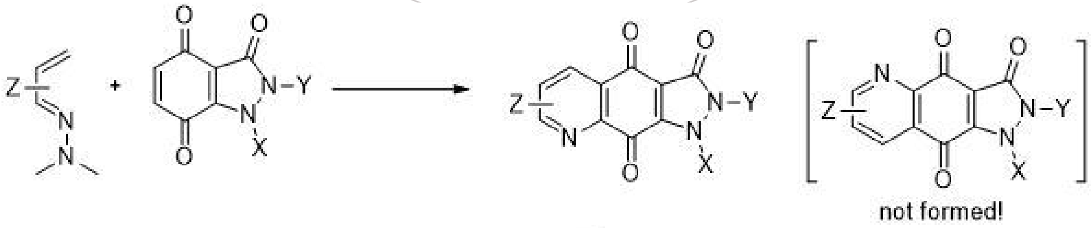
Exhibition Hall C FRI 11:00~13:00

Synthesis of pyrazolone-fused aza-naphthoquinone derivatives via regioselective hetero-Diels-Alder Reactions

Jeong Ho Kim, Hakwon Kim*, Kyungmin Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Diverse N-heterocycle-fused naphthoquinone (NQ) have been investigated for their various physiological activities. In our previous study, N-substituted pyrazol-3-one-fused naphthoquinone (NQ) derivatives were synthesized using a pharmacophore-hybridization approach and their biological activities were examined. In this study, pyrazol-3-one-fused aza-naphthoquinone derivatives were synthesized regioselectively through the hetero-Diels-Alder reaction of pyrazolone-fused benzoquinones with aza-diene. To confirm the structure of regioisomer, their single crystals were obtained and their exact structures were determined using X-ray crystallography, further supported by DFT calculation. Additionally, for investigating the biological activities of novel compounds, a basic biological evaluation, including toxicity, was investigated.



Poster Presentation : **MEDI.P-282**

Medicinal Chemistry

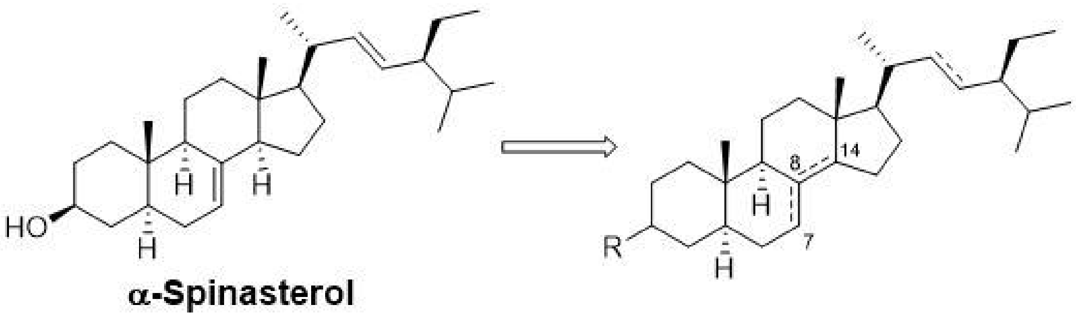
Exhibition Hall C FRI 11:00~13:00

Synthesis and anti-inflammatory activity of α-spinasterol derivatives

Hyejin Moon, Hong Joon Yoon[1], Hakwon Kim[2,*]

Department of Chemistry, Kyung Hee University, Korea
[1]*chemistry, Kyung Hee University, Korea*
[2]*Department of Applied Chemistry, Kyung Hee University, Korea*

α-Spinasterol, isolated from *Stewartia koreana* leaves, has been identified as a potent anti-inflammatory compound. The interest in such α-spinasterol has led to extensive research; however, the difficult in obtaining α-spinasterol from the natural source made the situation challenging. While several methods for the synthesis of α-spinasterol are known, issues like low yield and poor reproducibility have persisted. In this study, we explored an efficient method for synthesizing α-spinasterol from commercially available stigmasterol. Additionally, to synthesize compounds in which double bonds were moved to positions 8 and 14 through the hydrogenation of α-spinasterol, and each derivative was synthesized. Furthermore, we introduced various functional groups at position 3 instead of the OH group to synthesize novel α-spinasterol derivatives. These derivatives were evaluated for anti-inflammatory activity, and some compounds showed more potent anti-inflammatory activity than α-spinasterol


HO
H
H
H
α-Spinasterol
R
8
14
7
H
H

Poster Presentation : **MEDI.P-283**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Drug synthesis to solve the side effects caused by drug interactions between prohibited concomitant medications

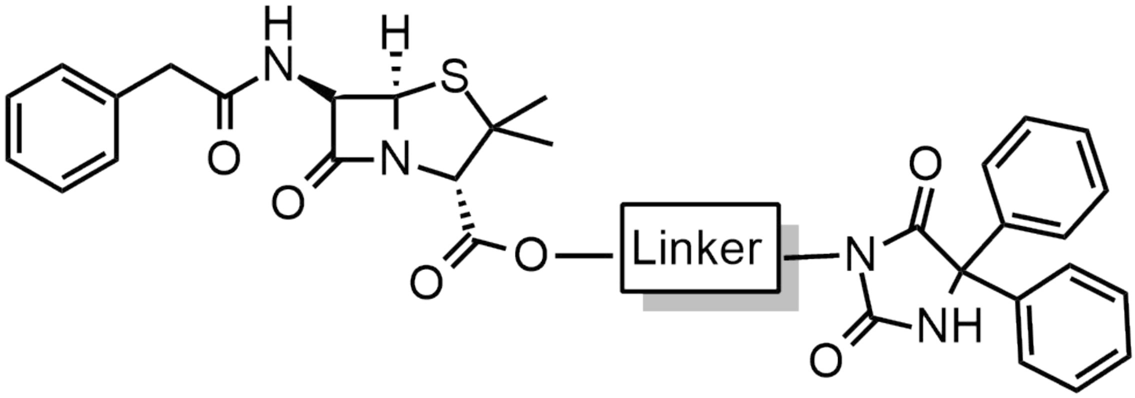
Jia Kim, Miyeon Choi, Taejun Park, Jaemin Bae, Chang Wook Jung, Sunggi Lee[1,*], Byunghyuck Jung[2,*]

Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Dept. of Physics and Chemsitry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

[2]*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Patients who suffer from several diseases are required to take multiple drugs at the same time. However, it sometimes happens that simultaneous dose of different drugs results in the deterioration of drug's activity or severe side effects. For example, it is well known that co-administration of phenytoin (5,5-diphenylhydantoin), an anticonvulsant, and penicillin G (benzylpenicillin), an antibiotic, causes side effects due to physicochemical reasons. To minimize the negative effects by co-administration, we hypothesized that the side effects come from the undesired intermolecular interactions between different drugs as well as competitive interactions of each drug to target proteins. Hence, our idea of solving this problem is a connection between two different drugs with a proper linker to minimize the aforementioned undesired interactions. As a model study, we chose phenytoin and penicillin G as intervening drugs and tried to synthesize new molecules bearing the moieties of phenytoin and penicillin G with a link. A variety of linkers from simple aliphatic chains to substituted aromatic rings were introduced between two drug molecules. Then, we will investigate bio-activities of these molecules as an anticonvulsant and an antibiotic.


Linker

Poster Presentation : **MEDI.P-284**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Efficient estimation of protein solvation free energy and vibration entropy using graph neural networks

Yeseul Oh

pharmacy , 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-285**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Characterization study of Apixaban microsphere

Surin Min, Sung-Joo Hwang*

Yonsei University, Korea

The purpose of this study is to characterize apixban microsphere. < Methods >Characterization study A differential scanning calorimetry study was carried out for microspheres by Q2000 DSC (TA Instruments, New Castle, USA). The Fourier transform infrared spectroscopy spectra data of apixaban, RG 502H, caprylic acid, and all 15 Runs were analyzed by using FT-IR spectrophotometer(FT-IR, Cary 630, Agilent technologies Ltd, Santa Clara, USA). DSC Apixaban exhibits a distinctive endothermic peak at 238°C, widely recognized as its melting point. In contrast, PLGA showcases a broader endothermic peak at 38°C, which corresponds to its glass transition temperature (Tg). All samples displayed a merged peak, where the PLGA co-polymer peak slightly shifted to the left of the apixaban melting peak. FT-IR Apixaban's FTIR spectra displayed characteristic peaks at 1592 cm^{-1} (associated with N-H bending) and 3310 cm^{-1} (indicating N-H stretching). The FTIR spectra of PLGA showcased distinct peaks at various wavenumbers, including 1748 cm^{-1} (attributed to C=O stretching), 1194 cm^{-1} (related to C-O stretching), and 2948 cm^{-1} (representing C-H stretching). Similarly, caprylic acid displayed a peak at 1705 cm^{-1} (related to C=O stretching).< Conclusion > Key attributes of the microspheres, including entrapment efficiency, drug loading, mean particle size, SPAN, as well as the D10, D50, and D90 values of the particles, were chosen as parameters of interest. *Acknowledgements We would like to extend our sincere gratitude to Sharif Md Abuzar for significant contributions to this paper. Their insights, feedback, and assistance were invaluable throughout the research process. Their dedication and support greatly enhanced the quality of this work. We are truly thankful for their involvement and collaboration.

Poster Presentation : **MEDI.P-286**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

DTC0630, a fluorescent imaging probe selectively targeting gingipains of Porphyromonas gingivalis

Aizhan Abdildinova, Lizaveta Gotina[1], Yun Kyung Kim[2,*], Ae Nim Pae[2,*]

Brain Science Institute, Korea Institute of Science and Technology (KIST), Korea
[1]*Department of Bio-Medical Science and Technology, University of Science & Technology, Korea*
[2]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

Porphyromonas gingivalis, a gram-negative oral anaerobe, is a major pathogen of severe adult periodontitis and was detected in more than 70% of periodontal disease patients. It produces arginine- and lysine-specific cysteine proteinases, gingipains, that are responsible for at least 85% of the total proteolytic activity of the various strains of P. gingivalis. Rapid and accessible detection and tracking of gingipains and P. gingivalis via fluorescence imaging would be advantageous for the diagnosis of periodontal diseases. In this work, we developed a thiol-reactive fluorescent probe DTC0630 with more than 6-fold fluorescence activation upon incubation with P. gingivalis. DTC0630 is equipped with a thiol-reactive Michael-acceptor warhead that targets the catalytic cysteine residue of gingipains. In vitro analysis demonstrated the selectivity of the fluorescent probe toward P. gingivalis and gingipains as well as the dose-dependent response of the fluorescence intensity for both probe and gingipain concentrations. NMR model study and molecular docking study with simplified thiols demonstrated a plausible binding mechanism of the probe at the binding pocket suggesting the formation of the 1,4-adduct and potential reversibility of the process. TD-DFT calculations supported our hypothesis as the oscillator strength calculations indicated the probability of the S0 → S1 transition is higher for the DTC0630 thiol adduct than the ligand unbound state. Moreover, DTC0630 demonstrated gingipain inhibitory activity and P. gingivalis growth inhibition showing its potential as a theragnostics tool.

Poster Presentation : **MEDI.P-287**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Discovery of novel β-arrestin-biased S1P1 agonists for the treatment of Multiple Sclerosis

Chang Yong Lee, Jushin Kim[1], Jong-Hyun Park[1], Sang Min Lim[1], Ki Duk Park[1], Jae Yeol Lee[2], Ae Nim Pae[1,*]

Kyung Hee University, Korea

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

[2]*Department of Chemistry, Kyung Hee University, Korea*

Multiple sclerosis (MS) is a chronic, progressive autoimmune disease which causes demyelination of the CNS. The non-selective Sphingosine-1-phosphate (S1P) receptor modulator, FTY720, binds to S1P1, 3, 4, 5. In Human clinical trials, it is associated with diverse side effects such as hypertension by S1P3 agonism. Our rationale of developing novel selective S1P1 receptor Agonist is to be lower the circulating lymphocytes more efficiently by internalization of S1P1 on lymphocyte. We designed and synthesized S1P1 receptor agonists with selectivity against S1P3 receptor via in silico docking study on S1P1 receptor crystal structure. The synthesized compound KKPY2045 showed remarkable in vitro activities (Ca2+ signaling assay, EC50=13.8 nM, β-arrestin assay, EC50=2.37 nM) with sparing activity against S1P3 receptor. Furthermore, the compound KKPY2045 decreased the lymphocytes in the peripheral lymphocyte count (PLC) assay and ameliorated the clinical score in the experimental autoimmune encephalomyelitis (EAE) model.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-288**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Organosilica-Based Hydrogen Sulfide Nanogenerator

Yerim Lee, Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea

Hydrogen sulfide (H_2S) has been implicated as a key signaling molecule that mediates many physiological and pathological processes. Hydrogen sulfide has been shown to inhibit tumors and is considered a potent tumor treatment. Therefore, we established an organosilica-based hydrogen sulfide nanogenerator, named sulfur-ball, in which many polysulfides are incorporated on the surface of the organosilica nanoparticles. Polysulfides on the nanoparticles can be triggered by glutathione (GSH) to release H_2S, and the structure of polysulfides can control the concentrations of H_2S. Polysulfide-coating on the surface of sulfur-ball was achieved by our previous method, which is the reaction between pyridyl disulfides and trialkyl silanethiols in aqueous media, and the capacity of releasing H_2S was determined by a fluorescent probe. In addition, we demonstrated the generation of H_2S from the sulfur-balls in cells.

Poster Presentation : **MEDI.P-289**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Direct Conversion of Biothiols to Persulfides

Yuri Lee, Baskar Selvaraj[1], Jaeho Kim, Subin Ham, Maniriho Olivier, Jae Wook Lee[2], Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea

[1]*natural product research center, Korea Institute of Science and Technology, Korea*

[2]*Natural Product Research Center, Korea Institute of Science and Technology, Korea*

Reactive sulfur species (RSS), sulfur-containing molecules such as hydrogen sulfide (H_2S), persulfide (RSSH), and polysulfide (RSS_nR'), play essential roles of redox regulation in the physiological and pathological processes. Among them, persulfides have attracted increasing attention because they display both nucleophilicity and electrophilicity and are more powerful reductants than their biothiol counterparts. Therefore, persulfides may exhibit more potent pharmacological effects than other thiols, which show vasodilation, cardiovascular health, angiogenesis, inflammantion, and neuroprotection. However, very limited in vitro studies have been performed due to the lack of persulfide donors and their instability. Here, we demonstrated thiirane-based small molecules that can convert biothiols such as cysteine and glutathione into the corresponding persulfides, like enzymes that produce persulfides. In addition, we investigated these molecules' unique ability to promote direct persulfhydation, a process of converting a protein thiol (protein-SH) to the corresponding protein persulfide (protein-SSH), and regulate the activity of a protein. This new approach would allow a complement to current chemical tools for the investigation of the behavior of persulfides in living systems.

Poster Presentation : **MEDI.P-290**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Rational Design, Synthesis and Biological Evaluation of Novel Ionizable Pantothenic Acid-Medicated Lipid Materials for mRNA, DNA, and siRNA Delivery

Faisal Muhammad, Eun-Kyoung Bang[1,*], Gyo chang Keum[2,*]

Organic chemistry, University of Science & Technology, Pakistan
[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*
[2]*Chemoinformatics Research Center, Korea Institute of Science and Technology, Korea*

- Withdrawal -

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-291**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Discovery of Lead Compounds for the Treatment of Progressive Supranuclear Palsy by Controlling 4R Tauopathy

Da Yeon Jeong, Ae Nim Pae[1,*], Yongseok Choi, Yun Kyung Kim[1,*], Lizaveta Gotina[2]

Biotechnology, Korea University, Korea

[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

[2]*Department of Bio-Medical Science and Technology, University of Science & Technology, KIST School, Korea*

The hyperphosphorylation, misfolding and subsequent accumulation of the microtubule-associated tau protein into abnormal filamentous intracellular inclusions occurs in over 20 neurodegenerative diseases, deemed tauopathies. Among them, progressive supranuclear palsy (PSP) is a late-onset primary tauopathy, whose symptoms include loss of balance, slow or stiff neck and limb movement, difficulty controlling eye movement, and cognitive impairment. It is classified as a 4R predominant tauopathy, in which tau inclusions contain a high ratio of the tau isoform with 4 microtubule-binding domains. Unfortunately, there is no available treatment for PSP and currently only short-lasting symptomatic relief is provided to patients. Therefore, we pursued the discovery of novel tau-targeting therapeutic drug candidates for the treatment of PSP, focusing our efforts on 4R tau aggregation inhibitors. To find 4R tau-specific lead compounds, we first performed high-throughput screening based on the tau Bi-FC assay with in-house compound libraries and then carried out hit compound structural optimization to improve the in vitro activity and selectivity for 4R tau. Two compounds (DTC 2417 and DTC 2423) showed excellent activity and selectivity for 4R tau over 3R tau. Molecular dynamics simulations were used to identify potential binding sites of PSP tau fibrils and reveal the binding modes of hit compounds. Finally, we performed in vivo studies in the TauP301L–BiFC mouse model, in which the lead compounds improved motor function in the balance beam test and alleviated cognitive impairment in the Barnes Maze test. Further work on improving physico-chemical properties and toxicity should be conducted, nevertheless, the discovery of 4R tau specific aggregation inhibitors is a promising first step in developing clinical candidates for the treatment of PSP.

Poster Presentation : **MEDI.P-292**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Reliable Detection of DNase-I through Localized Surface Plasmon Resonance Using Uniform Gold Nanostructures Formed by Thermal Annealing of Weakly Adsorbed Gold Films

Chai Won Park, Donghyuk Seo, Wonhwa Lee*

Department of Chemistry, Sungkyunkwan University, Korea

Deoxyribonuclease-I (DNase-I), a representative endonuclease, is an important biomarker for the diagnosis of infectious diseases and cancer progression. However, enzymatic activity decreases rapidly ex vivo, which highlights the need for precise on-site detection of DNase-I. Here, a localized surface plasmon resonance (LSPR) biosensor that enables the simple and rapid detection of DNase-I is reported. Moreover, a novel technique named electrochemical deposition and mild thermal annealing (EDMIT) is applied to overcome signal variations. By taking advantage of the low adhesion of gold clusters on indium tin oxide substrates, both the uniformity and sphericity of gold nanoparticles are increased under mild thermal annealing conditions via coalescence and Ostwald ripening. This ultimately results in an approximately 15-fold decrease in LSPR signal variations. The linear range of the fabricated sensor is 20-1000 ng mL^{-1} with a limit of detection (LOD) of 127.25 pg mL^{-1}, as demonstrated by spectral absorbance analyses. The fabricated LSPR sensor stably measured DNase-I concentrations from samples collected from both an inflammatory bowel disease (IBD) mouse model, as well as human patients with severe COVID-19 symptoms. Therefore, the proposed LSPR sensor fabricated via the EDMIT method can be used for early diagnosis of other infectious diseases.

Poster Presentation : **MEDI.P-293**
Medicinal Chemistry
Exhibition Hall C FRI 11:00~13:00

Zwitterionic nanocomplexes facilitated by nitric oxide for enhanced treatment of severe respiratory infectious diseases through mucus-walking

Hye-Jin Lee, Jungbum Kim, 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.

Poster Presentation : **MEDI.P-294**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

Illudin S-Induced p53 Stabilization for Colorectal Cancer Treatment

Jinyoung Park, Jisun Kim, Wonhwa Lee*

Department of Chemistry, Sungkyunkwan University, Korea

Impairment of the p53 pathway is a critical event in cancer. Therefore, restoring p53 activity has become one of the most appealing anticancer therapeutic strategies. Here, we disclose the p53-activating anticancer drug illudin S, extracted from O. japonicus. Illudin S demonstrates a notable selectivity for the p53 pathway, restoring p53 and activating apoptosis and cell cycle arrest in CT26. Comprehensive docking simulations were used to predict the binding sites and chemical bonds between p53 and illudin S. As a results, illudin S directly binds to the p53 mdm2-binding domain, enhancing the protein's stability and transcriptional activity. The efficacy of illudin S as an anticancer agent toward cancer is further demonstrated in xenograft mouse models of colorectal cancer. Our results demonstrate that illudin S interacts with p53's N-terminal domain, a key site of MDM2-p53 binding characterized by hydrogen bonds. And it was also confirmed using surface plasmon resonance (SPR) analysis. The results establish the anti-cancer effects of illudin S, targeting the p53 transcription factor family of importance in human cancer, and provide a candidate for further development in cancer therapy.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MEDI.P-295**

Medicinal Chemistry

Exhibition Hall C FRI 11:00~13:00

[Withdrawal] Design and synthesis of Sirt6 activator for pancreatic cancer

Hak Hyun Lee, Noh Gyoungho[1,*], Yuhwan Mun[2,*]

Research Center for the Treatment of Rare Disease, Korea Research Institute of Chemical Technology, Korea

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

[2]*Department of Medicinal Bioscience, Konyang University, Korea*

- Withdrawal -

Poster Presentation : **MAT.P-296**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Tuning Core-shell Nanoparticles Interfacial Engineering for Plasmon-Enhanced Energy Conversion Performance

Lemma Teshome Tufa, Jaebeom Lee[*]

Chemistry, Chungnam National University, Korea

The properties of core-shell plasmonic nanomaterials, which result in hot charge-carrier generation, near-field enhancement, and injection, and elevation of local temperature, make them important candidates for electrocatalysis [1]. However, it remains unclear how plasmonic cores and shells influence catalysis performance. Herein, we present a plasmon-enhanced phocatalysis of hydrogen evolution reaction (HER) controlled by an interface-controlled core-shell structure of Au@Pd NPS. The Au@Pd core-shell structures demonstrated effective photoelectrocatalytic activities toward HER, whereas the catalytic activity was optimized by tuning the amount of Pd nanoparticle-coated Au nanoparticle surface. The results showed that the reaction rate decreased as the shell thickness increased. Core-shell structure-induced lattice strain and energetic hot electrons are attributed to such intriguing photoelectrocatalytic performances. The results provide a reliable means to design plasmonic core-shell bimetallic nanostructures with excellent catalytic activity and durability. Keywords: Tuning, Au@Pd Core-Shell Nanoparticles, Plasmon Enhanced, Hot Electrons, Lattice Strain, Hydrogen evolutionReferences 1.Shen, Y. Dai, X. Yu, K. Liu, S. Lin, Nano Energy, 95, 106977 (2022).

Poster Presentation : **MAT.P-297**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Advanced hybrid washing machine filters for effective elimination of microplastics and surfactants

Su Hyeon Son, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Emerging pollutants, microplastics (MPs), have emerged as a significant global concern. The highest percentage of MPs released into the environment occurs through daily laundry. The average weight of dreg obtained from 5 kg of laundry was 1.26 g/kg. According to energy dispersive X-ray (EDX) and thermogravimetric analysis (TGA) analyses, the dreg consisted of MPs (78.3–89 wt%, organic elements: C/O) and alien materials (11–21.7 wt%, inorganic elements: Al/Fe/Ca, etc.). Thus, to reproduce the real environment, alien materials (Fe3O4 and CaCO3) were added to various types of model MPs in the presence and absence of sodium dodecyl benzenesulfonate (SDBS) to test MP removal. Hydrophobic and hydrophilic MPs were generated upon laundering, accounting for 55–59% and 41–45% of MPs, respectively. We provide a novel approach to design a laundry filter system for the simultaneous removal of SDBS and hydrophilic/hydrophobic MPs.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-298**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Omega-3 fatty acid-enriched thermoreversible nanogel for prevention of capsular contracture

Mohuya Paul, Jungkyun Im[1,*]

Department of electronic materials, devices, and equipment engineering, Soonchunhyang University, Korea
[1]Department of electronic materials, devices, and equipment engineering, Department of Chemical Engineering, Soonchunhyang University, Korea

Numerous people around the world undergo breast reconstruction surgery every year. Even though it is one of the most popular plastic surgery procedures, this surgery comes with its drawbacks. The most common complication that patients face after the surgery is related to the formation of thick and hard capsules around the silicon implant, a phenomenon commonly known as capsular contracture. This leads people to go through multiple follow-up correctional surgeries. The exact reason for the formation of capsules around the breast tissue is debatable but it is found in previous studies that omega-3 fatty acid can potentially alleviate the formation of capsules, thus leading to less hassle to the patient and their families, both economically and physically.In this study, we prepared a thermoreversible nanogel containing fish oil as it is the crude source of omega-3 fatty acid (20-31%). Fish oil was first converted to an oil-in-water nanoemulsion which was then mixed with gelator molecule. For the gelator molecule, poloxamer 407 and poloxamer 188 were chosen as a mixture of these two polymers exhibit the ability to remain liquid at room temperature and turn into hard gel at 37 0C a.k.a. human body temperature, making a more straightforward application of the gel on silicon implant.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-299**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Study on Causes and Countermeasures for the Mass Death of Fish in Reservoirs in Andong-si

Keon Sang Ryoo

Department of Chemical and Biological Engineering, Andong National University, Korea

This study focused on determining the specific causes and prevention methods of mass fish deaths occurred in five reservoirs (Gagugi, Neupgokgi, Danggokgi, Sagokji, and Hangokji) in Andong-si. Various water quality parameters, such as phosphate phosphorus (PO4-P) and ammonium nitrogen (NH3-N), were analyzed and compared for each reservoir during the rainy season. Changes in the DO concentration and electrical conductivity (EC) were also observed at the inlet of the reservoir during raining using an automated instrument. In addition, DO was measured until the concentration reached 0 ppm in 10 min by adding livestock compost at various concentrations (0.05%, 0.1%, 0.3%, and 0.5% by wt.), where the concentration of the livestock compost represents the relative weight of rainwater. The DO concentration in the surface layer of reservoirs was 3.7 to 5.3 ppm, which is sufficient for fish survival. However, the fish could not survive at the bottom layer with DO concentration of 0.0-2.1 ppm. When the livestock compost was 0.3%, DO required 10-19 h to reach 0 ppm. Considering these results, it was confirmed that the DO in the bottom layer of the reservoir could easily change to an anaerobic state within 24 h when the livestock compost in the rainwater exceeds 0.3%. The results show that the direct cause of fish mortality is the inflow of excessive livestock compost into reservoirs during the first rainfall in spring. Therefore, to prevent fish death due to insufficient DO in the reservoir, measures should be undertaken to limit the amount of livestock compost flowing into the reservoir within 0.3%, which has been experimentally determined.

Poster Presentation : **MAT.P-300**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Recovery of Ammonium Nitrogen and Phosphate from the Piggery Wastewater as Struvite and Its Assessment for the Reduction of Water Pollution Through the Field Test

Keon Sang Ryoo

Department of Chemical and Biological Engineering, Andong National University, Korea

Excess N and P from the livestock manure applied to farm lands, have entered the water systems and poses a serious threat to the natural environment. Consequently, there has been recent awareness towards the management of livestock manure and its related fields. In this study, piggery wastewater was collected from a piggery in Pohang city, Korea. At 800℃, thermal decomposition of a natural stone, magnesite (MgCO3), yielded powered MgO with particle sizes ranging between 10 to 100 μm. Furthermore, NH4+-N and PO43–-P were recovered as struvite precipitates from the piggery wastewater, by adjusting the pH with MgO and H3PO4. At pH 10, the recovery efficiencies of NH4+-N and PO43–-P were found to be 86.1% and 94.1%, respectively. Using an X-ray Diffractometer (XRD), the struvite in the precipitate was confirmed to be consistent with standard pure struvite. Further, the purity of the struvite precipitate was analyzed using an energy dispersive X-ray (EDX) and thermal gravimetry-differential thermal analysis (TG-DTA), and found to be between 79.2% and 93.0%. Additionally, struvite-containing piggery wastewater and sawdust were mixed in a weight ratio of 2.5:1 and processed into a mature compost. The newly manufactured compost passed all quality standards required for first-class graded livestock composts. Moreover, this compost was sprayed directly onto the soil at the test site, and various parameters of the soil's effluent, such as total organic carbon (TOC), total nitrogen (T-N), total phosphorus (T-P), and dissolved oxygen (DO), were analyzed and measured. Based on these results, it is determined that the newly manufactured compost can more significantly reduce water pollution than commercial compost

Poster Presentation : **MAT.P-301**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Manufacture of electrospun porous PLA fiber-type film coated with CMC and its anti-adhesion efficiency in white mice

Keon Sang Ryoo

Department of Chemical and Biological Engineering, Andong National University, Korea

The electrospun polylactide (PLA) anti-adhesion fiber-type film coated with carboxymethylcellulose (CMC) was manufactured and evaluated for its usability through animal experiments. The PLA anti-adhesion film developed in this study is an adhesion preventive film of a double composite structure with both hydrophobicity and hydrophilicity. This film has the anti-adhesion effect due to hydrophobic PLA that do not melt easily in the body and at the same time is easily attached to the surgical site by hydrophilic CMC that reacts easily to body fluids and changes quickly to mucus. In this study, the diameter and the pore diameter of the PLA fiber and thickness of PLA film made by electrospinning was 0.2–0.4, 1–10, and 30–50 μm, respectively. Through observation of surface structure (5000 magnification), the most suitable concentration of CMC to maintain pores on the PLA film as much as possible is 0.5% wt/vol. The CMC content in the PLA film coated with 0.5% wt/vol of CMC was measured to be 5.41% wt/wt and its tensile strength was about 2.92 times higher than that of the noncoated PLA film with CMC. The porosity of CMC-coated PLA film (5.41% wt/wt) was found to be 76.4%. In the animal experiment, 20 white mice (10 as a control group and 10 as an experimental group) were used to determine the degree of adhesion prevention. As a result of observing adhesion and anti-adhesion between the cecum and the peritoneum by performing Ushaped laparotomy on white mice at the third week after surgery, the incidence of adhesion in the control group was 90%, whereas the experimental group was 20%.

Poster Presentation : **MAT.P-302**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Wet-based cylindrical air filters for simultaneous removal of PMs and VOCs

Won san Choi*, Youngju Jung[1]

Department of Chemical & Biological Engineering, Hanbat National University, Korea
[1]Chemical Biological Engineering, Hanbat National University, Korea

An innovative wet-based air filter was implemented, comprising an inner cylindrical hydrophilic filter and an outer hollow cylindrical hydrophobic filter, installed within an output chamber that is filled with water. The WAF with water (WAF-WW) showed outstanding recyclability for up to 100 cycles with consistent long-term performance and low pressure drops, which were better than those of commercial HEPA filters (H13), at similar PM2.5 concentrations (1,700 μg/m3) and air velocities (1 m/s). The WAF-WW also exhibited excellent recyclability up to the 50th cycle with fast and complete removal of HCHO gas at very low concentrations (0.08–4.98 ppm). Furthermore, since small PM0.3/PM2.5 particles and total volatile organic compound (TVOC) that are hardly filtered by air filters can be easily and quickly removed by the WAF-WW due to the water filter, this is another extraordinary benefit of the wet process over the dry process.

Poster Presentation : **MAT.P-303**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Preparation and characterization of V2O5-decorated carbon nanotubes as a visible-light active photocatalysts

Gyuyeong Go, Hyun Chul Choi[1,*]

Department of chemistry, Chonnam National University, Korea

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

Water pollution is one of the crucial environmental issues because the organic and toxic chemical compounds in wastewater have affected human and animal life in the ecosystem. The semiconducting oxide-based photocatalysis is one of the most favorable and efficient green techniques for degrading harmful inorganic and organic pollutants from wastewater. Vanadium pentoxide (V2O5) holds ample potential as an effective photocatalyst because of its appropriate bandgap energy for the visible light absorption (~2.8 eV), long-term chemical- and photo-stability, and strong oxidizing power. However, the conventional V2O5 powder has the high rate of photo-induced electron-hole recombination, which limited the formation of surface radicals within the photocatalyst, resulting in low photocatalytic efficiency. In this study, we designed a noble photocatalysts of carbon nanotube (CNT) supported V2O5 nanoparticles (V2O5-CNT) by a simple sol-gel method. The as-prepared V2O5-CNT shows the highest degradation efficiency against the rhodamine B molecule, which could be attributed to the rapid generation of charge carriers under visible light irradiation.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-304**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

One-Pot Design of $CsPbClBr_2$ Blue Perovskite Quantum dot Control for High-Purity Luminescence with Precursor Stoichiometry

Jin Young Kim, Dong Hwan Wang*

College of ICT Engineering School of Integrative Engineering, Chung-Ang University, Korea

The synthesis of perovskite-based blue emitting colloidal particles is valuable for several applications as it can apply the superior properties of the composed materials related to multiexciton generation. However, cesium-based perovskite quantum dots (PQDs) can be obtained through a complex manufacturing process, mainly by preparing Cs-oleate at high temperatures. However, we would like to propose a facile synthesis method to obtain $CsPbClBr_2$ QDs. We investigated suitable precursors and solvents to obtain them in the ambient condition. However, additional by-products were identified during the synthesis process, and by minimizing and removing them, we succeeded in obtaining blue PQDs with a narrow FWHM. The obtained $CsPbClBr_2$ QDs used stoichiometric precursors and exhibited a quantum yield of 70.55% and a FWHM of 14 nm. In addition, no discoloration was observed and high PL intensity was maintained for 400 hours. Additionally, as a result of confirming the stability of the perovskite structure by making a double layer of $CsPbClBr_2$ QD solution and deionized water, it was confirmed that blue light emission was maintained even after 15 days. Through these results, we present a one-pot design to synthesize high-purity blue light-emitting PQDs.

Poster Presentation : **MAT.P-305**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Dual emissive Mn-Doped Lead Halide Perovskite Nanocrystals for Background Interference Suppressed Latent Fingerprint Detection

Hyejin Choe, Haksung Jung[1], Junsang Cho[2,*]

Chemistry, Sungshin Women's University, Korea
[1]*Quantum Technology Institute, Korea Research Institute of Standards and Science, Korea*
[2]*School of Chemistry and Energy, Sungshin University, Korea*

Diverse strategies have been developed to visualize latent fingerprints (LFPs) since it is undetectable by naked eye at crime scenes. Among them, fluorescence approach has been emerged as an attractive method that can permits high-resolution fluorescence image of LFPs. However, application of fluorescent probes for LFPs detection is challenging due to wearisome processing, low selectivity, and high background interference. Here, we demonstrate highly efficient, sensitive, and background free LFP detection with Mn-doped lead halide perovskite (CsPb(Cl1−yBry)3) nanocrystals (NCs). Incorporating of Mn into cesium lead halide perovskite NCs with different composition of halide can provide dual-emissive features. CsPb(Cl1−yBry)3 NCs are dried to use as a fluorescent powder in powder dusting methods. They retain their high quantum efficiency during preparation of solid-state nanopowders due to their high optical stability. Highly efficient fluorescence of solid-state nanopowders can visualize obvious ridge structure of LFPs with level 1 – 3 features of LFP. The dual emissive nature of the nanopowders allows background interference free high-resolution fluorescence imaging of LFPs. The combination of high quantum efficiency and dual emissive nature of Mn-doped CsPb(Cl1−yBry)3 NCs have great potential for forensic science.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-306**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Revealing the Role of Defects in Ternary Cu–In–Se Quantum Dots for Boosting Photoelectrochemical Hydrogen Generation

Shi Li, Su Il In[1,*], Jiwoong Yang[2,*]

Energy science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, China

[1]*Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

[2]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Eco-friendly Cu–In–Se quantum dots (CISe QDs) are promising materials for solar-energy conversion due to their low toxicity, tunable bandgap, and high absorption coefficient. However, defects in semiconductor QDs has been poorly controlled, especially for the ternary semiconductor QDs because of the synthesis challenges. We present the defect engineering of CISe QDs for efficient solar-energy conversion by controlling the Lewis acid–base reactions between metal halide–oleylamine complexes and oleylammonium selenocarbamate. The CISe QDs with In/Cu=1.55 exhibit the most outstanding photoelectrochemical hydrogen generation with the excellent photocurrent density up to 10.7 mA cm-2 (at 0.6 VRHE). Our results provide an effective method to control defects in ternary QDs and the resulting QDs have great potential as efficient solar absorbers for photoelectrochemical hydrogen generation.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-307**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Double-layer transfer printing strategy for high-resolution red/green/blue perovskite nanocrystals patterning.

Kiwook Kim, Jiwoong Yang[1,*]

Department of Energy science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

For evolution to next-generation displays, high-resolution of red/green/blue (RGB) pixels is definitely required with high color purity. Herein, our research team introduce a double-layer transfer printing method with metal halide perovskite nanocrystals and organic charge transport layer. The mechanical properties of optimized organic layer enable to prevent the internal cracking of the perovskite nanocrystal films during the patterning process. We achieve high-definition RGB pixelated patterns with a transfer yield of ~100% and resolution of up to 2250 pixel per inch (PPI). The perovskite light-emitting diodes (PeLEDs) by transfer printing show outstanding electrical characteristics with remarkable external quantum efficiency (~15.3%) and bright luminance. This approach provides the potential of transfer printed PeLEDs for high-resolution full-color displays.

Poster Presentation : **MAT.P-308**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Impact of Surface Characteristics of Quantum Dots on the Efficiency of Intaglio Transfer Printing Process

Kyunghoon Lee, Jiwoong Yang[1,*]

Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Semiconductor nanocrystals, known as quantum dots (QDs), have significant attention for their potential in display devices; achieving precise high-resolution patterns is crucial for their application. Dry transfer printing, a popular method for this purpose due to its ability to maintain QD properties, is employed. However, the impact of surface ligands on this process remains insufficiently understood, despite its importance. Herein, we explore how surface ligands influence intaglio transfer printing, focusing on CdSe@ZnS QDs with organic ligands (ranging from C8 to C18) and inorganic ligands (I^-). The results reveal that QDs with longer organic ligands exhibit a 100% patterning yield, even for patterns narrower than 10μm. Patterning yield diminishes as ligand chain length decreases, with the lowest yield observed for QDs with I^- ligands. Surface energy analysis and finite element simulations identify two key factors contributing to printing failure mechanisms: inadequate adhesion leading to improper pickup of QDs with inorganic ligands and a propensity for internal crack formation, particularly in QDs with short-chain ligands. These findings unveil previously unknown challenges in the intaglio printing process and hold promise for enhancing QD applications in next-generation high-resolution displays.

Poster Presentation : **MAT.P-309**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

MXene-based zwitterionic polymer hydrogel with adhesive, electrically conductive, and viscoelastic properties

Yiluo Hu, Taehun Chung, Jaewon Choi, Younsoo Kim*

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

Hydrogels containing conductive two-dimensional (2D) materials have received considerable attention due to their valuable properties, such as high electrical conductivity and mechanical strength. Among the 2D materials, MXene ($Ti_3C_2T_x$) exhibits excellent dispersibility, rich surface chemical functional groups, and excellent electrical conductivity.This study fabricated a conductive and viscoelastic hydrogel based on a three-dimensional cross-linked structure by dipole-dipole interaction between MXene and zwitterionic polymer. The uniformly distributed $Ti_3C_2T_x$ MXene was synthesized by chemically etching aluminum atoms on MAX ($TiAlC_2$) in an HCl/LiF mixed solution. Then, hydrogels were fabricated by simultaneous exfoliation of aqueous MXene and copolymerization of zwitterionic monomers (SBVI) through microwave irradiation. The obtained MXene/Poly(SBVI) hydrogel exhibits excellent adhesive strength and electrical conductivity, and in particular, mechanical properties such as viscoelasticity of the hydrogel have properties similar to those of living tissue. Therefore, the future of MXene/Poly (SBVI) hydrogels holds tremendous potential as novel and innovative bioelectrode materials.

Poster Presentation : **MAT.P-310**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Halide Ion Mixing across Colloidal 2D Ruddlesden-Popper Perovskites: Implication of Spacer Ligand on Mixing Kinetics

Junsang Cho*, Seonhong Min

School of Chemistry and Energy, Sungshin University, Korea

Halide ion exchange seen in metal halide perovskites provide a substantial opportunity to control their halide composition and corresponding optoelectronic properties. Halide ion mixing across colloidal 3D perovskite nanocrystals have been extensively studied while the mixing with colloidal 2D counterparts remain underexplored. In this study, we demonstrate the halide ion exchange kinetics across colloidally stable 2D Ruddlesden-Popper layered bromide (Br) and iodide (I) perovskites using two different spacer ligands such as aromatic phenethyl ammonium (PEA) *versus* linear butyammonium (BA). The halide exchange kinetic rate constant (k_{mix}), as determined by tracking time-dependent absorbance changes, indicates that Br/I halide mixing in 2D PEA-based perovskites (2.7×10^{-3} min^{-1}) occurs at an order of magnitude slower than in 2D BA-based perovskites (3.3×10^{-2} min^{-1}). Concentration (~1 mM to 100 mM) and temperature-dependent (50 to 80°C) kinetic studies further allow for determination of activation barrier for halide ion mixing across the 2D layered perovskites with 75.2 ± 4.4 kJ/mol (2D PEA) and 57.8 ± 7.8 kJ/mol (2D BA), respectively. The activation energy reveals that the type of spacer cations plays a crucial role in controlling the halide ion mobility and halide stability due mainly to the internal ligand chemical interaction within 2D structures.

Poster Presentation : **MAT.P-311**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Real-Time Imaging of Moisture-Induced Degradation of Quantum-Sized Nanocrystals through Amorphous Intermediates

Soyeon Lee, Jungwon Park[1,*], Jiwoong Yang[*]

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

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

Mechanism study of water-induced degradation of quantum-sized semiconductor nanocrystal is necessary because exposure to moisture is inevitable in their applications. Several studies investigated the way to control stability of the nanocrystals, because they are more vulnerable to water and oxygen exposure compared to their bulk counterparts due to high surface-to-volume ratio. However, the conventional liquid cell challenges in effectively observing real-time degradation process due to their structural limitations. In this work, we observe real-time degradation of quantum-sized CdS nanorods using an advanced liquid cell, GDLC (Graphene double-liquid-layer cell) which can observe the reaction from the initiation. Formation of non-crystalline domain is captured at the initial stage of the decomposition process. The non-crystalline region gradually grows, and the entire region become amorphous. We can obviously distinguish crystalline and non-crystalline domain with atomic-scale imaging capability by using GDLCs. The decomposition process without electron beam confirm that this process does not essentially require electron beam. We envision that our research can contribute to further comprehension of the deformation of nanocrystals by diverse factors.

Poster Presentation : **MAT.P-312**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Phase Transition Mechanisms of 2D CdSe Quantum Nanosheets Induced by Off-Stoichiometry at Atomic-Scale

Soyeon Lee, Jungwon Park[1,*], Jiwoong Yang[*]

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

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

Semiconductor crystal phase transitions have been applicated to a diverse systems, because the inherent material properties are significantly influenced by their structure. However, understanding the mechanisms of phase transitions in quantum-sized semiconductors at the atomic level remains a challenge. In this presentation, we introduce the phase transition phenomenon in two-dimensional (2D) CdSe quantum nanosheets induced by off-stoichiometry. The dynamic pathways of the phase transition are observed by in-situ transmission electron microscopy. The atomically flat CdSe nanosheets in wurtzite-phase are transformed into zincblende-CdSe nanosheets. Both experimental and theoretical approaches are used for analyzing the transformation process. The $(11\bar{2}0)$ basal planes of wurtzite-CdSe nanocrystals after the loss of Se atoms is similar with (001) basal planes of zincblende-CdSe, driving the phase transition. Furthermore, we can observe unconventional phenomena caused by dynamic atomic rearrangements including domain coalescence and separation during this structural transformation. This study can enhance our fundamental comprehension of the mechanisms governing semiconductor nanocrystal phase transitions, providing an intuitive insight into the transformation process.

Poster Presentation : **MAT.P-313**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of monodispersed InP quantum dots and their ZnSe/ZnS shell growth for bright and narrow band edge emission

Hyekyeong Kwon, Jiwon Bang[*], Ju Ho Kim[1]

Incheon National University, Korea

[1]*Dept. of Chemistry, Incheon National University, Korea*

Colloidal quantum dots (QDs) have garnered significant attention as promising candidates for wide color-gamut displays, owing to their exceptional photophysical characteristics. In particular, InP-based quantum dots with no inherent toxicity have emerged as a prospective choice for next-generation display and lighting applications due to their high absorption coefficients, broad color tunability, and excellent brightness. Nonetheless, the synthesis of InP quantum dots possessing a narrow emission linewidth and uniform particle size, which is critical for achieving high color purity in displays, presents a persistent challenge attributable to the unpredictable nucleation and ensuing growth kinetics of these quantum dots. In this study, we employ a heat-up method to form InP nano clusters at low temperatures, addressing batch-to-batch variations. Subsequent introduction of a Zn precursor to pre-formed quasi-stable InP clusters, followed by controlled heating, has not only elevated optical properties but also exerted a pronounced influence on nucleation and growth dynamics through the formation of Zn-P intermediate complexes in the reaction solution. The pre-formed InP clusters acted as a reservoir of continuous monomers, facilitating size-focusing growth of In(Zn)P quantum dots and enabling successful achievement of precise and uniform growth. In addition, by optimizing the coating conditions with ZnSe/ZnS double shells, we achieve brighter photoluminescence (PL) with a single exponential decay and a notably narrow the PL line width. By addressing the challenges associated with size distribution and placement reproducibility, it is expected to contribute to the realization of high-performance QD-based displays with improved color quality and brightness.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

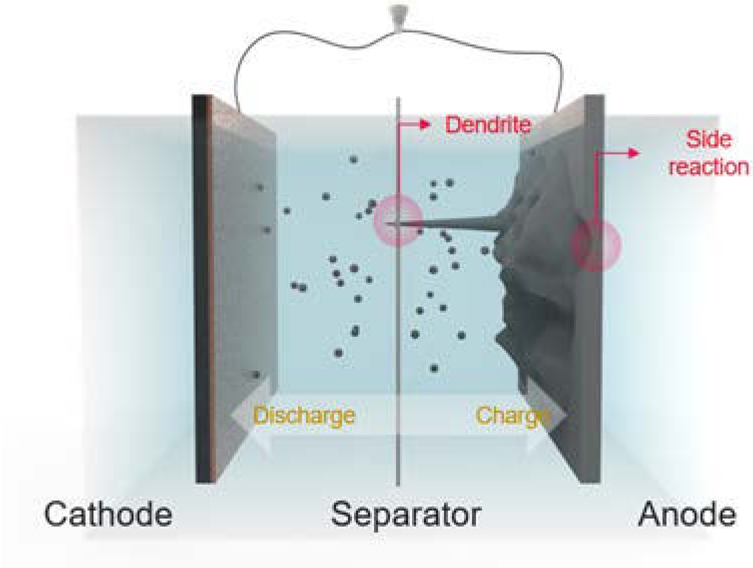
Poster Presentation : **MAT.P-314**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Study on the mechanism of SEI generated in aqueous Zn-Mn battery using ordered mesoporous manganese oxide by in-situ scattering X-ray

Chenglin Cui, Yelim Kwon[1], Ji Man Kim[1,*]

Chemistry, Sungkyunkwan University, China
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Lithium-ion batteries have the advantages of high working voltage, long life and high energy density, so they have always been the overlord in the battery market. However, LIBs also have other disadvantages, such as flammability, toxicity, and expensive lithium metal. And LIBs cannot work in the squeezed and bent state, so they cannot meet the future requirements for biocompatibility and flexibility. Moreover, the bottlenecks of flexible batteries, such as safety concerns and complex fabrication requirements limit the commercialization of flexible batteries. Recently as a new secondary battery, aqueous zinc-ion battery (AZIB) is being studied by many researchers. In terms of price, the price of lithium metal is much expensive than zinc metal. AZIBs have advantages lying in the high theoretical volume capacity of the metal zinc anode (5854 mAh cm 3), low standard redox potential (-0.76V) of Zn/Zn2+, non-toxic, low cost and high abundance. To study safe and environmentally friendly ZIBs, researchers have done a lot of research on ZIBs. On the cathode, dissolution of transition metals on the cathode as active substances hinders the stability and cycle life of the battery. Although there are many strategies to solve these problems, the performance of AZIBs is still not satisfactory in practical applications.


Dendrite
Side reaction
Discharge
Charge
Cathode
Separator
Anode

Poster Presentation : **MAT.P-315**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Synchrotron Based X-ray Analysis for Effects of Ordered Mesoporous Carbon as Selenium Support for Li-Se Batteries

Yelim Kwon, Chenglin Cui[1], Hansol Kim[1], Ji Man Kim[*]

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

The most widely used Li-ion battery has issues with low capacity, high cost and, the potential for explosion. Lithium selenium (Li-Se) battery is becoming one of the promising candidates for next-generation rechargeable batteries. It has high energy density and good kinetics. However, polyselenide is dissolved in the repetitive charging and discharging so it makes the capacity decrease, which is shuttle effect.Herein, we report on the use of ordered mesoporous carbon (OMC) to encapsulate selenium (Se/OMC) to reduce the shuttle effect by enabling the adsorption of dissolved polyselenide. It has superior electrochemical characteristics, such as increased capacity, improved cycle retention, and decreased resistance. Operando small angle X-ray scattering (SAXS) is a potent technique for analyzing the structure dynamics of mesoporous materials in real time during charging and discharging. Understanding the function of mesopores and the reaction mechanisms of selenium in OMC is possible by operating operando SAXS and ex-situ analysis by synchrotron-based X-ray absorption fine structure (XAFS).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-316**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

One-pot Synthesis of Mono- and Bimetallic Nanoparticles Using Acrylic Monomer as Solvent, Reductant, and Stabilizer

Jeesu Moon, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

Noble metal nanoparticles have demonstrated various biomedical, optical, and electronic applications owing to their unique chemical and physical properties. However, their gram-scale synthesis remains a challenge. In this presentation, we demonstrate a method for the gram-scale synthesis of gold nanoparticles (AuNPs) using acrylamide (AAm) as a solvent. AAm possesses unique properties such as low melting temperature, high solvating power, and high solubility of its polymerized form (polyacrylamide; pAAm) in water. The viscosity of the AAm solvent can be chemically tuned by the polymerization of AAm and addition of a low-volatile diluent, which can stabilize highly concentrated as-synthesized AuNPs in gram quantities. The synthesized AuNPs are substantially stable and catalytically active under high ionic strength conditions owing to the pAAm protection on the particle surface. Further, the synthesis mechanism of the AuNPs has been thoroughly investigated. The versatility of the synthesis method is proved by synthesizing other mono-(Ag and Pd) and bimetallic (Au + Pd and Ag + Pd) nanoparticles using the AAm solvent with controlled viscosity. Importantly, the productivity of this synthetic strategy is the highest among the previously reported gram-scale synthesis methods of AuNPs. To the best of our knowledge, our study presents the use of acrylic monomer as a solvent for the gram-scale synthesis of noble metal nanoparticles for the first time. This study significantly extends the list of solvents with chemically tunable viscosity by including other acrylic reagents for nanomaterial synthesis, functionalization, and catalytic, optical, and electrical reactions under highly localized reaction conditions.

Poster Presentation : **MAT.P-317**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Electro/chemical deposition of C_{60} microcrystals on Cu(111) in LiCl-KCl eutectic molten salt

Rajmohan Rajendiran, Sun Hwa Lee[1,*], Rodney Ruoff[2,*]

Center for Multidimensional Carbon Materials Research, Institute for Basic Science, India

[1]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

[2]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

The C_{60} molecule has a large electron affinity and is electrochemically active. The growth of C_{60} films on metal surfaces on Cu(111), due to its small lattice mismatch, interests us. To date, room temperature C_{60} deposition on Cu(111) is carried out in aqueous and organic solvent mixtures. We are exploring depositing C_{60} at moderately high temperature in a molten salt eutectic. The C_{60} molecules have deposited on Cu(111) in the LiCl-KCl eutectic molten salt via an electro/chemical method at 600°C. SEM shows that the deposited C_{60} molecules are arranged in hexagonal-like shapes, and SEM-EDS shows a high carbon content. RAMAN spectra from these deposits suggest they are pristine C_{60}(s). Cross-sectional TEM images through several C_{60} microcrystal show them to be single crystals.

Poster Presentation : **MAT.P-318**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ligand free, well-dispersed quantum-sized tin(Ⅳ) oxide nanocrystals

Hooin Lee, Wongyun Byoun, Jung Tak Jang[1,*]

KCTech, Korea

[1]*Future Materials Research Institue / research team 2, kctech, Korea*

Tin(Ⅳ) oxide (SnO_2), the most stable oxide of tin, is the one of the n-type semiconductor materials that is widely used for quantum-dot light-emitting diodes (QLEDs), lithium batteries, supercapacitors, gas sensors. Especially, SnO2 as electronic materials is promising due to wide band gap energy and quantum-sized nanocrystals. However, it is not easy to control nano-sized particles, and there is a risk of lowering charge mobility owing to agglomeration of nanoparticles. We synthesized the nano-sized SnO_2 with a diameter 4±1 nm via hydrothermal method and that was well-dispersed in a variety of solvents without additional ligand treatment. It was treated by mild bead-milling that nano-sized SnO_2, nearly no defects of particles. Synthesized SnO_2 nanocrystals have a high stability as well as a quantum size effect. It can be looked forward to utilizing as the electron transport layer (ETL) for QLEDs.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-319**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Proton-conductive cobalt-based coordination polymer for memristive applications

<u>Uichan Lee</u>, Intek Song[1,*]

Andong National University, Korea
[1]*Department of Chemical and Biological Engineering, Andong National University, Korea*

Coordination polymers, especially porous ones, have attracted significant attention in recent years due to their diverse applicability in various fields including catalysis, gas storage, and conductivity. These unique materials offer advantages in design flexibility, allowing for tunable properties to meet specific requirements. One particularly promising application is in the realm of proton conduction, which is crucial for devices such as fuel cells and supercapacitors. The ability of porous coordination polymers to offer designable proton pathways offers potential advancements in this field. In this study, a cobalt-based coordination polymer was newly synthesized. The crystal images were obtained by scanning electron microscopy (SEM) and optical microscopy (OM). The crystal structure was confirmed by single crystal X-ray diffraction. In addition, the material can be spin-coated in the form of a film, and through this, electrical analysis confirmed that material exhibits proton conductivity as well as memristive properties.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-320**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Facile synthesis of size and shape-controlled silver nanoparticles

Seungmin Lee, Jaehee Song[*]

Department of Chemistry, Suncheon National University, Korea

Silver nanoparticles are widely applied in various fields due to their unique optical properties rooted in Localized Surface Plasmon Resonance (LSPR). These applications include optical filters, photothermal effects, energy harvesting from microwaves to visible light, improved cancer diagnosis, antimicrobial activities, flexible electronic devices, and colorimetric sensing. Among diverse silver nanostructures, two-dimensional silver nanoplates offer the ease of adjusting optical properties by controlling their aspect ratios and shapes. In this context, we induced planar twinning to synthesize silver nanoplates with a high yield by removing possible untwinned particles through peroxide-etchant synthesis. Dilution of the seeds led to the synthesis of larger nano-prisms with an absorption peak around 800nm. Silver nanoplates underwent shape transformation under both heated and photogenerated conditions. By utilizing a surfactant, CTAB, we were able to separate silver precursor from silver nano-plates, obtaining monodispersed nano-prisms.

Poster Presentation : **MAT.P-321**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Large-area Single Crystal Graphite

Dongho Jeon, Won Kyung Seong*, Rodney Ruoff[1,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

We have studied the growth of single-crystal graphite using the metal flux method with cobalt foil as the flux. Our home-built 4-inch crucible induction heating system achieves single crystal graphite growth above the cobalt-carbon eutectic temperature (1,325 °C). Real-time video recordings of experiments and measurement of emissivity changes of the cobalt foil during the heating process, help us begin to understand early stages of growth and growth mechanisms of the graphite film that is formed. From electron back-scattering diffraction (EBSD) in SEM, selected area electron diffraction (SAED) in TEM, Laue diffraction, and Raman spectroscopy, we characterized grain orientation, micro and bulk crystallinity, and the degree of graphitization. We are targeting measure physical properties of our graphite films in the near future.

Poster Presentation : **MAT.P-322**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Studying of mechanism of *Zn/meso-*MnO_2 battery system using X-ray absorption fine structure

Hansol Kim, Chenglin Cui, Yelim Kwon[1], Ji Man Kim[1,*]

Chemistry, Sungkyunkwan University, Korea

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

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. Manganese dioxide (MnO2) has been addressed by prior studies that Zn2+ can be inserted into crystal structure because it exhibits several crystal structures (α, β, γ, δ, and λ) with tunnel-type or layer-type structure. Understanding the energy storage mechanisms is essential for the one-step evolution of cathode materials for AZIB. However, these 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. This analysis method gives great insight into the complex energy storage pathway of MnO2 materials with various polymorphs. Based on this knowledge, we synthesized ordered mesoporous β-MnO2 through nano-casting method by using KIT-6 as hard-template and used it as the cathode active material. We performed ex-situ XAFS analysis at the states of charge during 2nd cycle to monitor energy storage mechanisms. These findings contribute to further understanding of the reaction mechanisms and capacity fading phenomenon and suggest practical strategies for next-generation zinc-ion batteries.

Poster Presentation : **MAT.P-323**

Material Chemistry

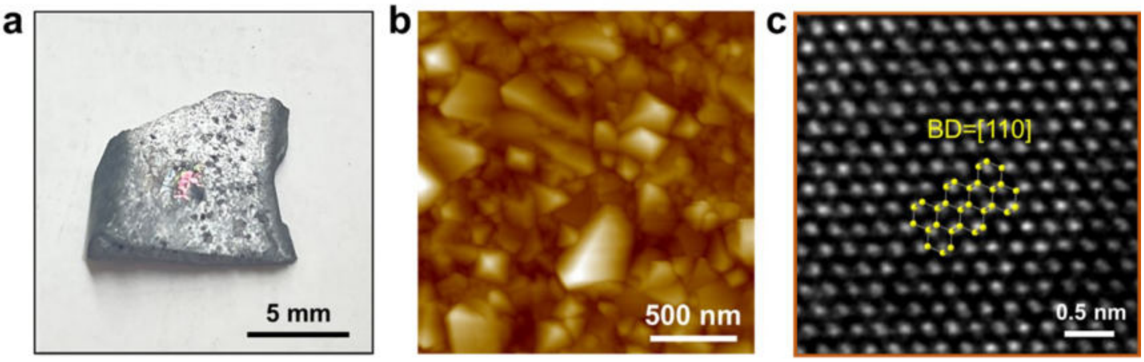
Exhibition Hall C FRI 11:00~13:00

Growing diamond in liquid metal at 1 atm

Yan Gong, Rodney Ruoff[1,*], Da Luo[2,*], Won Kyung Seong[3,*], Meihui Wang[4]

Center for Multidimensional Carbon Materials (CMCM) , Institute for Basic Science (IBS), Korea
[1]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*
[2]*Institute for Basic Science, Korea*
[3]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*
[4]*Center for Multidimensional Carbon Materials (CMCM) , Institute for Basic Science, Korea*

We discovered a new method to grow diamonds at the surface of liquid alloy metal (at the interface with the container of the liquid metal—a graphite heating element with a cavity machined into it). A metal mixture was placed inside this graphite crucible that was then resistively heated (Joule heating) until it was molten. Diamond particles are found embedded in the surface of the solidified metal piece (what had been the liquid metal) after cooling to room temperature. The temperature range in which diamonds grow seems to be relatively narrow. A variety of analysis methods prove growth of diamond by this new method (Raman, XRD, TEM, others). 13C-labeled methane proved that methane contributes carbon for the growth of these diamonds. Si-vacancy (Si-V) centers were found in the as-grown diamonds (strong photoluminescence peak at ~740 nm). Support from the Institute for Basic Science (IBS-R019-D1) is appreciated.


a
5 mm
b
500 nm
c
BD=[110]
0.5 nm

Poster Presentation : **MAT.P-324**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Carborane Superacids for Activation of Diamondoids

Bharat Ugale[*], **Sun Hwa Lee**[1], **Rodney Ruoff**[2,*]

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

[2]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

An acid with an acidity greater than that of 100% pure sulfuric acid, which has a Hammett acidity function (H0) of (-12), is classified as a superacid. Most strong superacids are prepared by the combination of a strong Lewis acid and a strong Brønsted acid. The carborane acids are a relatively new class of protic acids known for their strong yet gentle properties that allow the isolation of reactive cations e.g., H+, CH3+, CH5+, CH7+ and R3Si+ [1]. The icosahedral B12 cage of carborane may be the most stable cluster in all of chemistry! Having tangentially delocalized σ bonding (i.e., σ aromaticity) and with its σ bonds being the strongest in chemistry, the HOMO-LUMO gap in the CB11H12- cluster is much larger than that of σ aromatic systems. The high energy required for disruption of this icosahedral cluster gives the anion tremendous stability. Despite stability, the protruding B-H bonds are amenable to electrophilic substitutions in a manner similar to benzene. Thus the anions have very low nucleophilicity and are very weakly coordinating, i.e., strong yet gentle. Fully sp3-hybridized clusters of carbon which perfectly superimpose the diamond lattice framework and are hydrogen terminated are classified as diamondoids. Diamondoids are the smallest form of hydrogen terminated cubic diamond and they are highly symmetrical and strain free. Previously, superacids have been used to study proton transfer to adamantane and diamantane in solution phase [2, 3]. But the superacids used (such as Fluoroantimonic acid (2HF-SbF5) and Magic acid (FSO3H·SbF5)) were highly reactive leading to decomposition of the parent molecule, so superacids with an unreactive conjugate base are a better choice. High proton affinity (PA) and gas phase basicity (GPB) values [4] suggests it should be difficult and challenging for protonation of these exceptionally stable diamondoid molecules, such as by using general organic and inorganic acids.The synthesis of carborane acids and their solution and gas phase reactivity with diamondoids will be described. This research is supported by the Institute for Basic Science (IBS-R019-D1).References 1.Reed, C. A. H+, CH3+ and R3Si+ Carborane Reagents: When Triflates Fail. Acc. Chem. Res. 1998, 31, 133-139.2.Olah, G. A. Stable Carbonium Ions in Solution. New Superacid Solvents and Nuclear Magnetic Resonance Spectroscopy Permit Direct Study. Science 1970, 168, 1298-1311.3.Olah, G. A.; Lukas, J. Stable Carbonium Ions. Protonation of and Hydride Ion Abstraction from Cycloalkanes and Polycycloalkanes in Fluorosulfonic Acid-Antimony Pentafluoride. J. Am. Chem. Soc. 1968, 90(4), 933-938.4.Camacho-Mojica, D. C.; Ha, J. K.; Min, S. K.; Vianello, R.; Ruoff, R. S. Proton Affinity and Gas Phase Basicity of Diamondoid Molecules: Diamantane to C131H116. Phys. Chem. Chem. Phys. 2022, 24, 3470-3477.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-325**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and Characterization of Nickel Oxide Nanoparticles, and Observation of Changes in Magnetic Properties via Surface Modification

Wongyun Byoun, Hooin Lee, Jung Tak Jang[1,*]

KCTech, Korea

[1]*Future Materials Research Institue / research team 2, kctech, Korea*

The synthesis of metal oxide nanoparticles, including the calcination process, is a crucial issue in various material research fields due to the significant agglomeration that can occur post-calcination. Agglomerated nanoparticles can lead to inaccurate physical, optical, and electrochemical properties. In this report, we present a straightforward and high-yielding synthetic strategy for fabricating nickel oxide nanoparticles that exhibit superparamagnetic and ferromagnetic properties, while maintaining monodispersity within an organic solvent as well. Nickel oxide nanoparticles are easily synthesized through the sol-gel process, followed by calcination. To impart the hydrophobic surface of these nanoparticles, a ligand exchange is performed using alkyl silane. This modification enhances the particles' dispersibility in non-polar solvents. Vibrating sample magnetometer (VSM) analysis illustrates changes in the magnetic properties after surface modification. Nickel oxide has been extensively investigated for numerous optoelectronic devices owning to its excellent hole mobility and p-type semiconductor properties. These materials can serve as inorganic hole injection layers (HILs) in various applications, including perovskite solar cells and organic light-emitting diodes (OLEDs). We provide a comparison of the hole mobility of nickel oxide in hole-only devices (HOD). As a result, surface-modified particles demonstrate higher hole mobility compared to agglomerated particles.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-326**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Reaction of liquid gallium at near room temperature with a wide range of chemicals

Sudipta Bag, Bharat Ugale[1], Benjamin Cunning[2], Rajmohan Rajendiran[3], Sun Hwa Lee[2], Rodney Ruoff[4,*]

CHEMISTRY, Ulsan National Institute of Science and Technology, India

[1]*Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science, Korea*

[2]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

[3]*Center for Multidimensional Carbon Materials Research, Institute for Basic Science, Korea*

[4]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

We are studying the reaction of liquid gallium with a wide range of chemicals (i.e., reagents) at or close to room temperature. Our survey study of a very wide range of reagents is due to considering the bond enthalpies of Ga-N, Ga-O, and Ga-X (X=halogen) bonds, as well as the reported catalytic activation of C-H bonds by gallium. Powder (that is, solid) reagents are mixed with liquid gallium by ball milling. Liquid reagents are mixed with liquid gallium by cup horn sonication. To date, liquid gallium has reacted with almost all reagents (saturated and unsaturated hydrocarbons, cyclic hydrocarbons, aromatic hydrocarbons, heterocyclic aromatic organic compounds, reagents containing O, or N, halogenated or partially halogenated hydrocarbons, 43 reagents studied to date). In most cases a solid carbonaceous product forms while in some others, an 'oily' viscous product is obtained. We are finding that liquid gallium reacts with almost every reagent we have tried and near or at room temperature. NMR, Raman, energy-dispersive X-ray (SEM-EDS), X-ray photoelectron (XPS), infrared (FT-IR), electron energy loss (EELS), and UV-Vis-NIR spectroscopies; XRD; and SEM, TEM, and AFM microscopies, are being used to try to characterize the products. We appreciate support from the Institute for Basic Science (IBS-R019-D1)

Poster Presentation : **MAT.P-327**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Control of wetting properties for plasticizers in the PBXs

Huisu Shim, Kuktae Kwon, Seong Han Kim, Mingu Han*

Agency for Defense Development, Korea

Plastic-Bonded eXplosive (PBX) is composed of various components including explosives, metal fuels, pre-polymer, and plasticizer. The control of wetting between components is the key factor for manufacturing PBXs applying with a newly-developed substance.In this study, we synthesized candidates of new plasticizers with increased polarity by shortening of carbon chain from commonly used plasticizers, isodcyl pelargonate (IDP) and bis(2-ethylhexyl) adipate (DOA) in the PBXs and their interfacial tension with modified hydoxy-terminated polybutadiene (HTPB, prepolymer) were calculated by the Kaeble equation. In addition, their thermal characteristics were analyzed to confirm the minimum requirment as a PBX component.

Poster Presentation : **MAT.P-328**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Rational Design of Heterostructured Anode Materials: Layered Titanium Oxide and Covalent Organic Nanosheets for High-Rate and Durable Sodium-Ion Batteries

Seung-Min Paek*, Minseop Lee, Jin Kuen Park[1,*], Jae-Min Oh[2,*]

Department of Chemistry, Kyungpook National University, Korea
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*
[2]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Research on TiO_2-based anodes for sodium-ion batteries (SIBs) has received significant attention, but low electrical and ionic conductivity has limited their application in practical SIB systems. Various strategies have been proposed to address these issues, such as hybridization with carbon-based materials and nanoarchitectural engineering. This work presents a hierarchical hollow sphere (HS) structure formed from layered titanium oxide and covalent organic nanosheets (CONs). CON/TiO_2-HS was fabricated using the layer-by-layer (LBL) self-assembly method utilizing electrostatic interactions. In particular, due to the synergistic effect of CON used as a conductive matrix and TiO_2 with good structural stability, CON/TiO_2-HS exhibited excellent electrochemical properties, overcoming the limitations of TiO_2-based materials. The CON/TiO_2-HS electrode demonstrated a discharge capacity of 426.2 mAh g^{-1} after 600th cycles at 100 mA g^{-1}, which is noteworthy compared to conventional TiO_2-based electrodes. Therefore, hybridization and nanoarchitecture engineering with CONs and TiO_2 is a promising solution for advanced energy storage materials.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

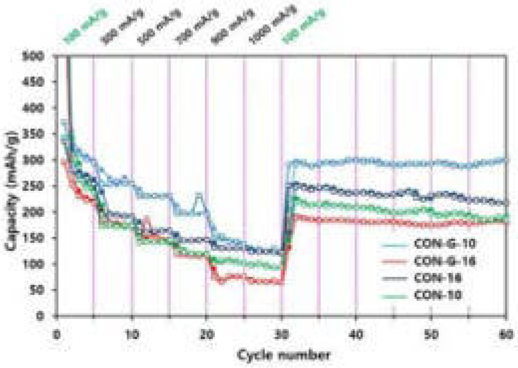
Poster Presentation : **MAT.P-329**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

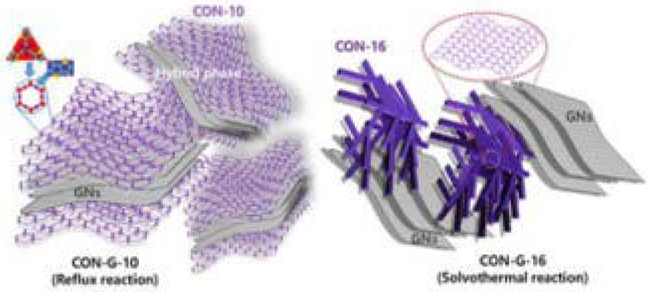
Electrodes in sodium-Ion batteries that take the form of nanosheets with organic/inorganic hybrid two-dimensionally for increased electrical conductivity toward steady and towering-performance

Na kyeong Lee, Jin Kuen Park[1,*]

department of chemistry, Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

To explore the impact of electrical conductivity in the energy-storage attributes of anode materials, graphene nanosheets (GN) that have highly conductivity are hybridized with covalent organic nanosheet; it is CON with shortly, through separate methods like solvothermal routes and reflux synthesis routes. The hybrid with reflux synthesis method shows overlapped 2D form, whereas hybrid with solvothermal routes take a shape with segregated phase that connection is diminished between CONs and GNs. These hybrids with facile synthesis routes are characterized completely, and the results uncovers their enhanced energy-storage property via the arrangement of a overlapped construction between CONs and GNs. Reflux synthesized hybrids showed greater ability of not only discharge capacity and but also rate capability than bare CONs. It means that reflux-synthesized hybrids have improved charge carrier transport. Therefore improvement of accessibility of sodium ions toward the hybrid surface has showed in the hybrids. This facile synthetic method can be enhanced to the fabrication for SIB system.


100 mA/g
300 mA/g
500 mA/g
700 mA/g
900 mA/g
1000 mA/g
100 mA/g
Capacity (mAh/g)
500
450
400
350
300
250
200
150
100
50
0
0
10
20
30
40
50
60
Cycle number
CON-G-10
CON-G-16
CON-16
CON-10


CON-10
Hybrid phase
GNs
CON-G-10
(Reflux reaction)
CON-16
GNs
GNs
CON-G-16
(Solvothermal reaction)

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-330**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Preparation of three-dimensional layered double hydroxide filters by 3D printing

Tae-Hyun Kim, Jeong Hoon Park*

Accelerator and Radioisotope Research Section, Korea Atomic Energy Research Institute, Korea

In this study, we prepared a three-dimensional (3D)-structured adsorbent utilizing 3D printing technology and a layered double hydroxide (LDH) nanoparticles. To prepare the 3D filter materials, polylactic acid (PLA) pellets were transformed into filaments using a filament extruder and then printed by a fused deposition modeling (FDM) 3D printer. Then, MgAl-LDH was synthesized onto the surface of the 3D filter by coprecipitation method. Scanning electron microscopy (SEM) images revealed that the incorporated LDH nanoparticles were observed on the surface of the PLA filter from smooth to rough. The adsorption characteristics of the produced PLA-LDH filter were examined using methyl orange (MO) as a model contaminant. Batch experiments showed that the MO adsorption efficiencies of the PLA-LDH filter shows enhanced efficiency (59%) compare to the pristine PLA filter (0%). The SEM images after adsorption showed that the LDH was well maintained on the filter surface during the adsorption. Adsorption kinetics and isotherms confirmed the suitability of the pseudo-second-order and Freundlich models, respectively. Furthermore, a laboratory-scale column built with the PLA-LDH filter was successfully operated for 8 h, and the experimental results were well-fitted by the Thomas column model. Thus, the PLA-LDH filter which had not been explored in previous LDH hybridization studies, is an effective adsorbent material for removing anionic dyes.

Poster Presentation : **MAT.P-331**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of durable column material for $^{68}Ge/^{68}Ga$ generator system

Jun Young Lee, Jeong Hoon Park[*]

Accelerator and Radioisotope Research Section, Korea Atomic Energy Research Institute, Korea

The column materials are the key component for the radioisotope generator system. Especially inorganic ion exchangers were studied extensively for the application to the adsorption and desorption of parent and daughter radionuclides, due to their selectivity for specific ions, acid resistance, and long-term stability. In particular, we synthesized chitosan-based TiO_2 adsorbent via a physical trapping method as a durable $^{68}Ge/^{68}Ga$ generator column material.In order to observe the morphology and crystallinity of chitosan-based TiO_2 at the microscale, these materials were characterized by SEM-EDX and X-ray diffraction. Physisorption capacity of N_2 gas adsorption and desorption were obtained using the Brunauer-Emmett-Teller. The adsorption/desorption studies exhibited a higher separation factor of $^{68}Ge/^{68}Ga$ with 0.1 M hydrochloric acid. The prepared chitosan-based TiO_2 showed acid resistance capabilities with >70% of ^{68}Ga elution yield and 10^{-3}~10^{-4}% of ^{68}Ge breakthrough. In particular, the labeling efficiency of DOTA and NOTA, using the generator eluted ^{68}Ga, was encouraging and confirmed to be >99%.These results suggest that chitosan-based TiO_2 column material has a high potential in the $^{68}Ge/^{68}Ga$ generator system.

Poster Presentation : **MAT.P-332**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

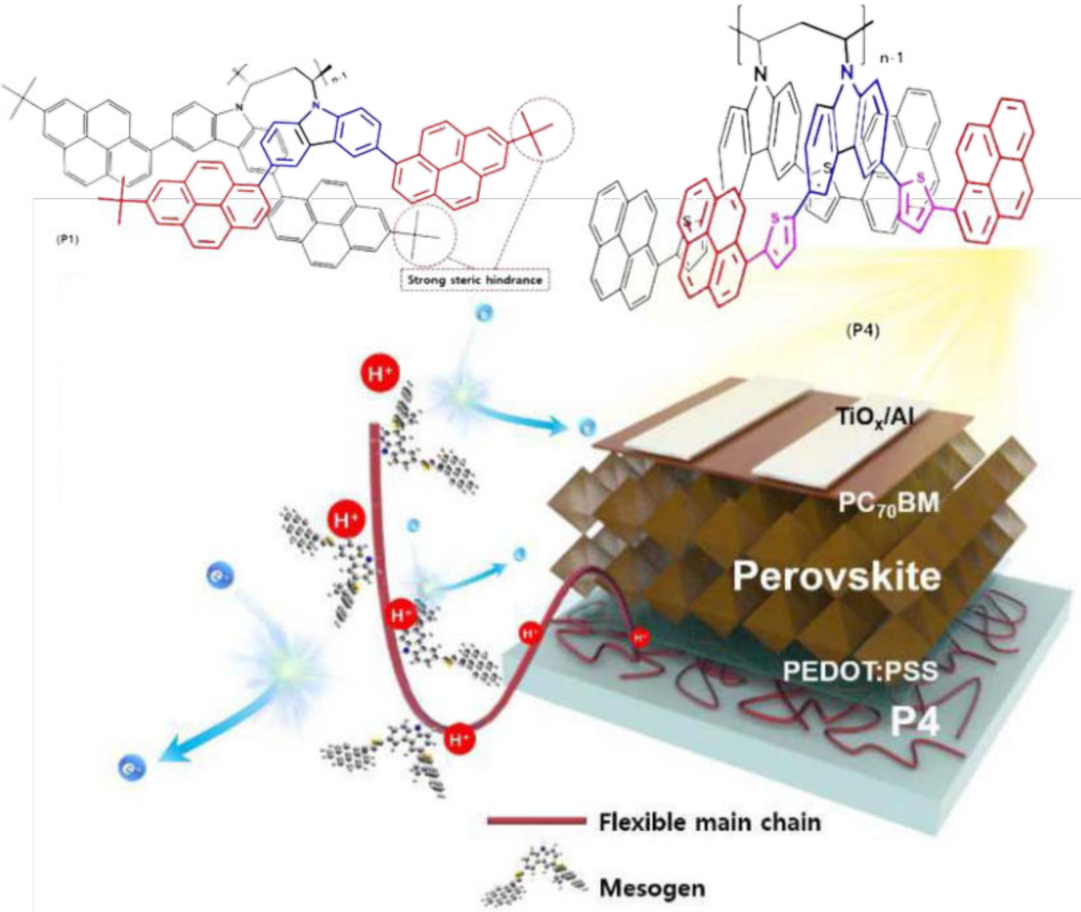
Using Pendant Polymer as Hole Transport Materials via Supramolecular Self-Assembly by Electron Withdrawing Functional Group

Byeong hwak Bae, Jin Kuen Park[1,*]

department of chemistry, Hankuk University of Foreign Studies, Korea

[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

PVK has high electronic properties which carbazole was attached like pendant (pendant polymer). We prepared PVK derivatives by attaching thiophene and pyrene to modify the highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) for efficient charge transfer in perovskite solar cell (PSC) and organic photovoltaic solar cell (OPC). To identify electronic properties of these materials, we compared various materials each other (P0, P1, P4). P4 which was attached thiophene and pyrene gradually shows low dark current and high charge transfer efficiency unlike to PVK(P0) and P1(t-butyl pyrene was attached). Because of bulky t-butyl motifs in P1, π-π conjugation of pyrene was not occurred in P1. Unlike at P1, P4 shows high electron conductivity because of supramolecular scale self-assembly structure through π-π conjugation effect of pyrene motifs. Through analysis of surface of these materials, P4 shows lowest trap density in film because P4 shows lowest roughness so it can improve contact area with each layers.


n-1
(P1)
Strong steric hindrance
N
S
(P4)
H⁺
TiOx/Al
PC70BM
Perovskite
PEDOT:PSS
P4
Flexible main chain
Mesogen

Poster Presentation : **MAT.P-333**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Effect of Polyvinylpyrrolidone (PVP) on Bismuth Catalysts for Electrochemical CO2 Reduction

Yongsu An, Yongju Lee[1], Duk-Young Jung[1,*]

chemistry, Sungkyunkwan University, Korea

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

Polyvinylpyrrolidone (PVP) is widely used in the synthesis of nanoparticles as a capping reagent. However, PVP does also block the active site of nano particles. Here, we report the difference of Faradaic efficiency (FE) for electrochemical CO2 reduction by bismuth catalysts according to presence of PVP in Bi particle synthesis. We prepare the Bi particle with and without PVP by sodium borohydride reduction and deposit the Bi on carbon paper using solution casting methods. The measured efficiency values of bismuth catalysts at -1.5V vs Ag/AgCl (sat. 3M KCl); ~95% of formate and ~2% of H2 without PVP, but ~82% of formate and ~15% of H2 with PVP capping, respectively. The detailed study of PVP effects on the electrochemical CO2 reduction offers opportunities for the design of novel electrocatalysts for carbon dioxide capture.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-334**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ethylene Glycol Based Crosslinking Agent Enables Photopatterning of Silver Nanowire Electrodes

Wanho Cho, BongSoo Kim[1,*]

Chemistry, Ulsan National Institute of Science and Technology, Korea

[1]*Department of Chemistry, UNIST, Korea*

We introduce an adaptable technique for fabricating transparent electrodes using silver nanowire networks through photopatterning. Despite the attractive properties of high optical transparency and electrical conductivity, the widespread adoption of transparent electrodes based on silver nanowire networks has faced difficulties due to the absence of a scalable micropatterning process. Our approach is based on photoinduced crosslinking and necessitates only a small amount of the photo-crosslinker (

Poster Presentation : **MAT.P-335**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Mechanistic Study of the Effect of Quantum Confinement and Triplet Energy Variation on Energy Transfer Efficiency Using Lead Halide Perovskite Nanocrystals

Yerin Kim, **Young-Je Kwark**[1,*]

Department of Green Chemistry and Materials Engineering, Soongsil University, Korea
[1]*Department of material sciences and engineering, Soongsil University, Korea*

The distinctive properties of nanocrystals arising from size, shape, and surface variations have a significant impact on their catalytic activity and interactions with reactants. This has generated considerable interest in research within this field. However, untangling the complex influences of energy gap changes and quantum confinement on photocatalytic performance remains challenging. In this study, we focused on halide perovskite nanocrystals (PNCs) as an adaptable model system with easily tunable photoelectric properties via crystal size and halide composition modifications. CsPbBr3 and mixed halide PNCs with emission peaks from 480 to 515 nm prepared by a hot injection process followed by post-anion exchange treatment. The photocatalytic properties of these PNCs were evaluated through [2+2] photo-cycloaddition reactions driven by triplet-triplet energy transfer. Smaller PNCs exhibited enhanced photocatalytic activity due to increased quantum confinement effects, resulting in efficient charge carrier separation and reduced recombination losses. Conversely, changes in the triplet energy had a relatively minor impact on photocatalytic activity.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-336**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Local Graphitization and Pore Blockage of Si@C Yolk-Shell Structure during Magnesiothermic Reduction

<u>Min seok Kang</u>, Seongchan Lee[1], Won Cheol Yoo[2,*]

Department of Applied Chemistry, Hanyang University, Korea
[1]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Herein, we first report that local graphitization and pore blockage of carbon shell of Si@C yolk-shell structure were identified during magnesiothermic reduction of SiO2@C core-shell structure. The microposority of carbon shell was completely blocked after magnesiothermic reduction and local graphitization of carbon shell was observed. Comprehensive physicochemical analyses were performed that such unexpected finding could be ascribed to the exothermic reduction nature of magnesiothermic reduction, resulting in graphitization and consequent pore blockage of carbon shell. As prepared Si@C yolk-shell structure exhibited outstanding capacitance of 1500 mAhg-1 (@100 cycles) with stable long term stability and prominent rate performance

Poster Presentation : **MAT.P-337**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Defect Engineering on UiO-66 for Glucose Conversion to Levulinic acid in Aqueous Condition

Sininat Boonmark, Asst. Prof. Dr. Sareeya Bureekaew[*]

School of Energy Science and Engineering (ESE) , Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand

The catalytic activity of highly robust UiO-66 was optimized through post-synthetic treatment method. To achieve this, UiO-66 was subjected to aqueous HCl solution, resulting in the defective framework containing an uncoordinated -COOH group. This treatment also induced the formation of a Lewis acidic accessible site, which was generated by the absence of the linker. The resulting defect-engineered UiO-66 exhibiting both Lewis and Bronsted acid characteristics enables to catalyze a multistep reaction for the conversion of glucose to Levulinic acid (LeV) under hydrothermal conditions. Moreover, an addition of NaCl as a promoter to the reaction can enhance the LeV yield.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-338**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Perovskite Nanocrystal as Triplet Energy Transfer Photocatalyst for [2+2] Cycloadditions of 4-Vinyl Aniline with Amine Functional Groups

Jeonghun Hyun, Young-Je Kwark*, Yerin Kim

Soongsil University, Korea

Direct utilization of long-lived triplet states using molecular chromophores for organic activation has been extensively explored. However, employment of triplet excitons from inorganic semiconductors is usually challenging, because such excitons are generally tightly confined within the semiconductor.Notable exceptions have been recently reported. Triplet energy transfer (TET) from CdSe quantum dots to organic molecules was observed, which subsequently induced chemo- and stereoselective [2+2] cycloaddition reaction that cannot be otherwise achieved by molecular photocatalysts.Lately, perovskite nanocrystals (PNCs) have been successfully adapted in TET photocatalytic reaction of organic molecules containing carboxylic acid groups. However, the TET reaction has not been successfully applied to organic molecules with amine functional group. The presence of the amine group is expected to result in distinct triplet energy states and interaction with PNCs in the organic molecules. The objective of this research was to utilize PNCs in the TET photocatalytic process involving the [2+2] cycloaddition reaction of 4-vinyl aniline. The effectiveness of PNCs in the photocatalytic reaction was assessed by comparing the yield and stereoselectivity with those obtained from the reaction involving 4-benzoic acid with carboxylic acid functionality.

Poster Presentation : **MAT.P-339**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhanced shielding against electromagnetic pulse and neutron shielding of unidirectional CNT mat-BN composites

YongBi Joo, Myung Jong Kim[1,*]

nanochemistry, Gachon University Global Campus, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

Carbon nanotube (CNT) mats have excellent mechanical properties, electrical conductivity and specific strength properties. It can be used in aerospace applications to reduce fuel consumption and as a fiber for spacesuits. However, CNT mats lack oxidation resistance and lack of neutron shielding ability, making them difficult to use in extreme environments such as space. Moreover, although CNT mats with a high CNT percentage are a promising form for producing nanocomposites, due to low tube-to-tube load transfer, poor CNT alignment, and physical defects created during fabrication, CNT mats have not achieved mechanical properties that can compete with CFRP. In order to solve this limitation, a composite with high oxidation resistance and thermal neutron shielding ability was coated with boron nitride (BN) on the UD structure CNT mat, in which nanotubes are arranged in one direction to more effectively resist stress in a specific direction. material was created. The BN coating was formed by thermal decomposition of borazine, a precursor, in the PECVD process. Through Raman and FTIR spectra, it was confirmed that the coating layer was h-BN. XPS analysis revealed the formation of new C–N covalent bonds at the interface between the CNT mat and the BN coating layer. TGA, tensile strength, and electromagnetic wave shielding ability tests were conducted on the composite materials. As a result, the composite material showed 130℃ higher oxidation temperature and 130% higher tensile strength than conventional CNT mats. In addition, electromagnetic wave shielding performance has been improved. It has great neutron shielding ability even with a small nano-scale coating thickness.

Poster Presentation : **MAT.P-340**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Cu-imidazole-resorcinol coordination compound and evaluation of its insecticidal activity against termites

Sanha Park, Jinkwon Kim[*], Seog Woo Rhee[*]

Department of Chemistry, Kongju National University, Korea

In this study, a new coordination compound was synthesized by the reaction of Cu^{2+} ion with a ligand having imidazole and resorcinol moieties, and the insecticidal activity of the Cu-imidazole-resorcinol coordination compound against termites was investigated. A ligand with imidazole and resorcinol moieties was synthesized by the reaction of 3,5-dihydroxybenzoic acid (3,5-DHBA) and 1,1´-carbonyldiimidazole (CDI), and a Cu-imidazole-resorcinol coordination compound was synthesized by the reaction of the purified ligand and Cu^{2+} ion. Functional groups of the compounds were analyzed using FT-IR spectroscopy, and molecular structures were analyzed using ^{1}H-NMR spectroscopy. Subterranean termites (Reticulitermes speratus) prevention experiments were carried out in choice and no-choice tests according to AWPA standard (E1-17). In the samples treated with the coordination compound, all termites died within 28 days, indicating 100% mortality. In conclusion, Cu-imidazole-resorcinol coordination compound showed performance as a very effective anti-termite agent.

Poster Presentation : **MAT.P-341**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Organo-Metallic Complex Inserted Montmorillonites Coated on Carbon Paper: A Novel Approach to Electrocatalysis for the Oxygen Evolution Reaction.

In Seon Lee

Chemistry, Kyung Hee University, Korea

With the acceleration of fossil fuel depletion and the environmental crisis, the development of highly efficient and low-cost energy sources that do not emit CO2 has become the top priority for addressing the global warming problem. Among the numerous promising research areas, water electrolysis is garnering significant attention as a viable process for producing green hydrogen energy—an environmentally friendly and renewable energy source. However, the 4-electron transfer process in the oxygen evolution reaction (OER) is characterized by inherently sluggish kinetics. To overcome this limitation and reduce the overpotential, active electrocatalyst is required. In this study, we synthesize effective electrocatalyst by inserting organo-metallic complex between the layers of montmorillonite (MMT) clay through host-guest reaction. Furthermore, facile synthesis process under ambient conditions enables high-throughput synthesis for industrial applications.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-342**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ordered Mesoporous Cobalt Oxides as a Negative Electrode for Li-ion Batteries: Electrochemical Properties

Jung-ho Lee, Yelim Kwon, Lee Jea Won[1], Ji Man Kim[*]

Department of Chemistry, Sungkyunkwan University, Korea

[1]*Sungkyunkwan University, Korea*

In recent days, as cutting-edge devices become more sophisticated, the battery performance is required to be higher. As a result, metal oxides having a capacity several times larger than that of carbon have attracted attention as a candidate for a nextgeneration secondary battery. CoO is very attractive anode material due to its relatively high theoretical capacity of 716 mAh/g. The nanostructured materials, especially mesoporous structure can play a leading role in electrochemical properties since its high surface area, large surface-to-volume ratio, and stable buffer effect against volume expansion. These characteristics provide especially anode materials with a lot of advantages which are fast ion/electron transfer, sufficient contact interface between active materials and electrolyte. Although bulk CoO maintains its own stable phase, mesoporous CoO gradually forms Co3O4 with Co metal through disproportionation process. It appears to be no significant difference in the TEM image by the disproportionation process, however, the changes in XRD and BET show that its nano pores and overall structure transform to another phase, and thus the electrochemical performance also changes.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-343**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Mercaptoamine-assisted efficient capture of ppm-level Hg^{2+} ions by FAU zeolite for water purification

Kang Min Lee, Hae Sung Cho[1,*], Changbum Jo[2,*]

Department of Chemical and Chemical Engineering, Inha University, Korea
[1]*Department of Chemistry, Chung-Ang University, Korea*
[2]*Center for Nanomaterials and Chemical Reactions, Inha University, Korea*

Utilizing adsorption to remove Hg(II) from wastewater has emerged as an energy-efficient method for water purification. Zeolite materials have attracted attention for this purpose due to their cost-effectiveness and stability. However, their efficiency has been hindered by limited adsorption capacity and selectivity towards Hg(II). In this study, we conducted investigations about the adsorption behavior of Hg(II) on commercially available FAU zeolites to enhance their adsorption capacity and selectivity for Hg(II). Our findings revealed that Hg(II) primarily interact with ion-exchange sites within the sodalite cages of the zeolite and hardly interact with ion-exchange sites within the supercages. To address this limitation, we introduced aminoethanethiol (AET, NH2-CH2CH2-SH) onto the pore walls of the supercages through dynamic acid-base interactions between the amine groups and bridging oxygen. This modification led to the introduction of free thiol groups that exhibited a strong capability to capture Hg(II) through the formation of Hg-S bonds. The resulting AET-grafted FAU zeolite demonstrated an impressive eight-fold increase in Hg(II) adsorption capacity and a 2.4-fold increase in Hg(II) affinity, all while maintaining a comparable adsorption rate to the pristine FAU zeolite. Notably, the AET-grafted zeolite exhibited remarkable selectivity in removing Hg(II) from solution containing multiple ions, whereas the efficiency of the unmodified FAU zeolite decreased significantly to around 10%. This distinct affinity of the thiol groups for Hg(II) combined with the dynamic acid-base interaction presents a versatile approach that can be extended to various zeolite systems. These modified zeolites hold promise for rapid and selective removal of Hg(II) in challenging purification scenarios.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-344**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and characterization of chromium-based coordination compounds reacting to ultraviolet light

Minjeong Kim, Minju Park, Intek Song*

Department of Chemical and Biological Engineering, Andong National University, Korea

Light-activated chemical reactions deepen our understanding of molecular properties and energy transitions. Such is crucial for harnessing solar energy and storing chemical energy. This research focuses on the light-activated reaction among chromium-based complexes. The solution was unresponsive to heat but reacted to ultraviolet (UV) light, undergoing a notable color change. This color transformation continued when the solution was placed in a dark chamber. To make sure if oxygen influenced this change, the experiment was replicated after degassing hexane. The consistent results confirmed that the UV exposure drove the solution's color shifts, suggesting UV's role in aiding the surpassing of activation energy. Such a color change implies the variation of coordination environments or other changes related to orbitals, which would allow for in-depth understanding in this field.

Poster Presentation : **MAT.P-345**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

CO_2 adsorption at low pressure using Zr-based metal-organic framework (UiO-67) functionalized with aminosilanes

Ha-Young Nam*, **Sung Hwa Jhung**[1,*]

Deartment of Chemistry, Kyungpook National University, Korea

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

Elimination of CO_2 from offgas of various sources is very significant against global warming. Here, we modified a Zr-based MOF (UiO-67), for the first time, with aminosilanes by utilizing μ-OH of the MOF in order to increase the performances in the CO_2 adsorption under low pressure of up to 100 kPa. Although the MOF does not have open metal sites (OMSs) that is effective in grafting Lewis bases like diamines, aminosilanes could be loaded facilely onto the MOF. Importantly, one modified UiO-67 showed a remarkable selectivity (based on ideal adsorbed solution theory, IAST $S_{CO2/N2}$) of 407 (at 100 kPa) which is 163 times as much as that of the pristine UiO-67. This IAST selectivity is higher than any result observed with MOFs having amino groups (excluding only a handful of results obtained from MOFs having very small pores). Moreover, the adsorbed quantity of CO_2 at 15 kPa over the modified UiO-67 was around 2.6 times that of the pristine UiO-67. Interestingly, the nitrogen content to show the most effective CO_2 adsorption (in both the selectivity and adsorbed quantity) was nearly constant of ca. 5.7 mmol/g irrespective of the type of applied aminosilanes; and there is little difference between primary and secondary amino groups in increasing the performances in CO_2 capture under low pressure. This study will pave the way to functionalize a MOF (although there is no OMS) with aminosilanes, providing a very effective adsorbent to capture CO_2 from offgas, especially under low pressure.

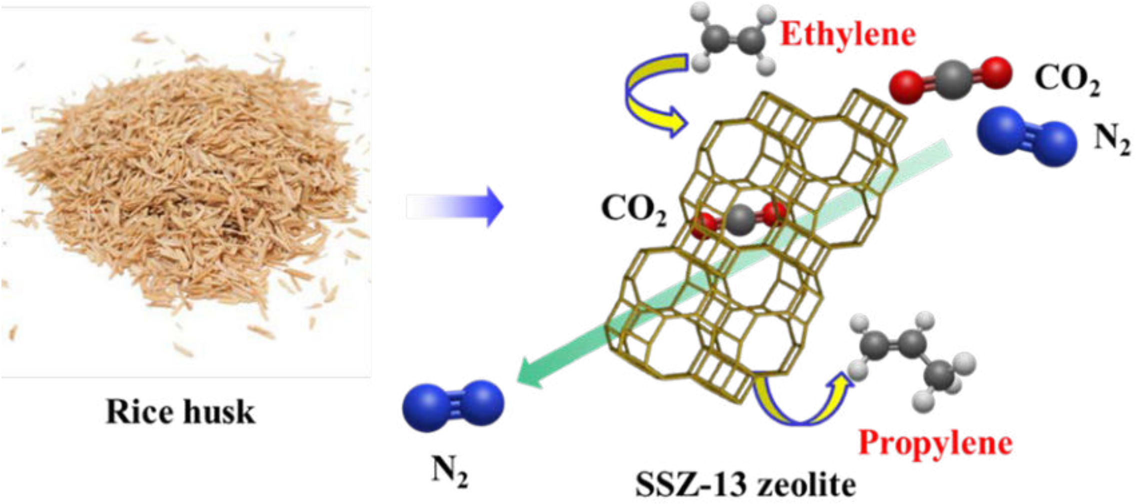
Poster Presentation : **MAT.P-346**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Propylene production from ethylene and carbon dioxide adsorption with SSZ-13 zeolites prepared from calcined rice husk as silica source

Jeongbin Lee, Sung Hwa Jhung*

Department of Chemistry, Kyungpook National University, Korea

DeNOx, CO_2 capture/separation, methanol-to-olefin conversion, and direct conversion of ethylene to propylene (DCEP) can be done by using SSZ-13 zeolites, with a small pore of 8-membered rings. Although the synthesis of SSZ-13 has been done for a long time and is useful for some applications, further development in the synthesis is required to reduce the production cost or to optimize the preparation. On the other hand, the utilization of waste is important for our sustainability. In this study, SSZ-13 zeolite was synthesized using rice husk-derived silica, for the first time, in order to prepare SSZ-13 at a low cost and utilize agricultural byproduct in zeolite synthesis. Via this research, it was found that SSZ-13s could be synthesized readily by using rice husk-derived silica even without seed crystals. Synthesis at 180 ℃ for 5-7 d leads to SSZ-13 from the gel with a wide range of silica/alumina ratios. Prepared SSZ-13 in proton form, together with a commercial SSZ-13, was utilized in DCEP and CO_2 adsorption at low pressure. The two H-SSZ-13s showed very similar performances in DCEP and CO_2 capture, showing an agricultural waste or byproduct, rice husk, can be successfully utilized in the preparation of SSZ-13 zeolites.


Rice husk
Ethylene
CO_2
N_2
CO_2
Propylene
N_2
SSZ-13 zeolite

Poster Presentation : **MAT.P-347**

Material Chemistry

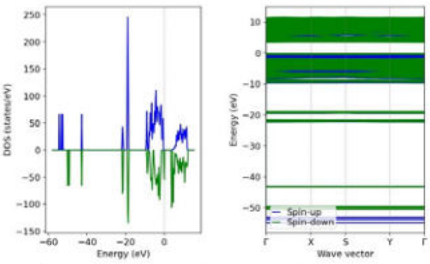
Exhibition Hall C FRI 11:00~13:00

Computational Analysis of Lithium Iron Phosphate Cathode Material Doped with Silicon or Nitrogen for Enhanced Electronic Conductivity

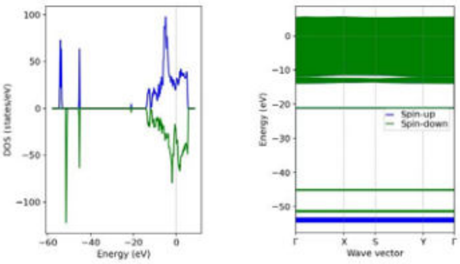
Yelak Abebe

Nano Convergence Technology , Pusan National University , Korea

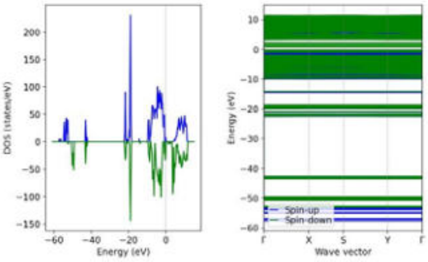
Lithium iron phosphate (LFP) is a promising cathode material for lithium-ion batteries due to its superior safety profile and environmental friendliness. By virtue of the atoms being arranged in an orderly manner, the olivine crystal structure of LFP has intrinsic stability. The strong iron-phosphate bond also contributes to the crystal system's stability. The battery technology does, however, have some important disadvantages, including a reduced energy density and comparatively slower charging rates. Using density functional theory (DFT), this study explores substitutional doping of silicon in lieu of phosphorous and nitrogen in place of oxygen atoms to enhance the electrochemical performance of LFP cathode material. The band gap of the LFP crystal was reduced from 3.660 eV to 0.001 eV by doping 6.25% silicon atoms, whereas the band gap was decreased to 1.133 eV by doping 1.56% nitrogen atoms. The increased electronic conductivity has been directly correlated with the improved charging rate.



DOS (states/eV)
250
200
150
100
50
0
−50
−100
−150
−60
−40
−20
0
Energy (eV)
Energy (eV)
10
0
−10
−20
−30
−40
−50
Spin-up
Spin-down
Γ
X
S
Y
Γ
Wave vector



DOS (states/eV)
100
50
0
−50
−100
−60
−40
−20
0
Energy (eV)
Energy (eV)
0
−10
−20
−30
−40
−50
Spin-up
Spin-down
Γ
X
S
Y
Γ
Wave vector



DOS (states/eV)
200
150
100
50
0
−50
−100
−150
−60
−40
−20
0
Energy (eV)
Energy (eV)
10
0
−10
−20
−30
−40
−50
−60
Spin-up
Spin-down
Γ
X
S
Y
Γ
Wave vector

Poster Presentation : **MAT.P-348**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Regulation of the formation of calcium carbonate polymorphs using 1*H*-imidazole-4,5-dicarboxylic acid as an additive

In Soo Koo, Jungkoo Lee[1], Jinman Kim[1,*], Seog Woo Rhee[*]

Department of Chemistry, Kongju National University, Korea

[1]*Department of Green Smart Architectural Engineering, Kongju National University, Korea*

In this study, we carried out experiments in which additives regulate the formation of calcium carbonate polymorphs in the process of forming solid calcium carbonate by the reaction of calcium ions and carbonate ions in aqueous solutions. After adding 1*H*-imidazole-4,5-dicarboxylic acid (H_3IDC) to an aqueous calcium chloride solution to form a calcium-IDC complex, an aqueous solution of sodium carbonate was added dropwise while maintaining a constant pH at room temperature. Calcium carbonate was synthesized under various conditions by varying the pH and concentration of H_3IDC, and the obtained phases and the ratio of each phase were analyzed by powder XRD. The vibrational modes of functional groups were identified by FT-IR, and the morphologies of calcium carbonates were identified by FE-SEM. In the absence of additives, typical calcite crystals were obtained under high pH conditions (pH ~12) and spherical vaterite crystals were obtained under low pH conditions (pH ~8). In the case of experiment using H_3IDC as an additive, a spherical vaterite phase was obtained even under high pH conditions. Under high pH conditions, amorphous calcium carbonate formed at the initial stage of the reaction forms calcite crystals through repeated dissolution-recrystallization processes. In this process, added H_3IDC is capped on the surface of amorphous calcium carbonate, preventing the dissolution-recrystallization process and leading to the formation of the metastable vaterite phase. After the reaction is complete, the additive remains dissolved in the aqueous solution and can be removed in a washing process. This study suggests a new method in which calcium ion-complexing additives regulate the formation of calcium carbonate polymorphs.

Poster Presentation : **MAT.P-349**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Elimination of aromatic diamines from water using metal-organic frameworks functionalized with a nitro group

Gyudong Lee, Sung Hwa Jhung[1,*]

Chemistry, Kyungpook National University, Korea

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

Elimination of aromatic diamines such as methylenedianiline (MDA) and p-phenylenediamine (PPD) via adsorption was firstly investigated with nitro-functionalized metal-organic frameworks (MOFs, MIL-101(Cr)-NO_2). The MIL-101 (Cr)-NO_2 showed much better performances in the removal of MDA and PPD, in both adsorption capacity and kinetics, than any other adsorbents. For example, MIL-101(Cr)-NO_2 had a much higher maximum adsorption capacity for MDA (1111 $mg\cdot g^{-1}$) than activated carbon (208 $mg\cdot g^{-1}$) or a reported adsorbent (391 $mg\cdot g^{-1}$). Based on experimental results, hydrogen bonding (especially, via the formation of a 6-membered ring (6-MR) between -NO_2 of the adsorbent and -NH_2 of the adsorbates) could be suggested as the main mechanism to interpret the noticeable adsorption of the diamines. Importantly, this is the first example to confirm that MOFs with nitro group can be a competitive adsorbent to remove organics composed of amino group, especially via making 6-MR through hydrogen bonding. Higher adsorption of MDA than that of PPD over MIL-101(Cr)-NO_2 might be explained with π-π interaction between aromatic rings (π-lean aromatics of MOF and π-rich aromatics of the adsorbates). Moreover, MIL-101(Cr)-NO_2 could be recycled after simple washing, suggesting the potential use of the MOF in adsorptive purification of contaminated water with organics with amino groups.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-350**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Carbon Isotope Enrichment from the Electromigration of ^{12}C and ^{13}C in Cobalt and Nickel

Alisher Sultangaziyev, Sun Hwa Lee, Dongho Jeon, Da Luo, Won Kyung Seong*, Rodney Ruoff[1,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials / Department of Chemistry / Department of Materials Science and Engineering, IBS CMCM / UNIST, Korea*

Electromigration is the movement of impurities and even metal atoms within a metal under the influence of electrical current. We are studying the electromigration of carbon isotopes in cobalt and nickel by introducing mixtures of different ratios of ^{12}C and ^{13}C. Co and Ni bars (designed for this experiment and thus machined to a specific geometry) were first annealed at 1400 ˚C in a 1:3 Ar:H_2 atmosphere for a long time which achieves: removal of impurities that might adversely affect the carbon electromigration, and significant grain growth. The carbon source was prepared by ball-mixing and then placed in a 'pocket' located in the middle of the Co and Ni bars. Under either AC or DC current this pocket region is heated up close to the carbon-metal eutectic temperature. The geometry of the Co and Ni bars ensures temperature gradients from its center towards each of the two (water-cooled) electrodes that drive the diffusing (migrating) carbon to accumulate at the lower temperature region leading to precipitation of a graphite film. AC yielded a perfectly symmetric distribution of precipitated graphite "to the left and to the right" of the center line. But under DC, precipitation of a graphite film is observed only on one side of the bar, causing us to think of electromigration. Raman mapping of the graphite region is used to quantify the isotope ratio, as the G peak frequency depends on the $^{12}C/^{13}C$ ratio. The results of the Raman mapping and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) measurements show isotopic enrichment of ^{12}C relative to ^{13}C for both Ni and Co. *We appreciate the support from the Institute for Basic Science (IBS-R019-D1).*

Poster Presentation : **MAT.P-351**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Study of three-dimensional porous structure and its evolution of zeolite-templatedcarbons

Madi Arsakay, Alisher Fatkhulloev, Sun Hwa Lee[1], Won Kyung Seong[1], Rodney Ruoff[2,*]

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science, Korea
[1]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*
[2]*Center for Multidimensional Carbon Materials, IBS CMCM / UNIST, Korea*

3D architectures of porous carbons composed of trivalently-bonded carbon attract interest for basicscience as well as for potential use in catalysis, adsorption, mechanical devices, electronics, andenergy storage, among others. One way to obtain such structures is to utilize “top-down” synthesis bytemplating the carbon product using existing porous and periodic (crystalline) solids, such aszeolitesOur studies have included obtaining atomic-resolution images with integrated differential phasecontrast scanning transmission electron microscopy (iDPC-STEM) of both the zeolite and the carbonstructure inside each zeolite channel, as well as the progression from the initial to the final stages ofgrowth of carbon networks inside zeolite channels by electron microscopy, gas adsorption,thermogravimetric analysis, X-ray diffraction, Raman spectroscopy, and solid state nuclear magneticresonance. We (MA, AF, SHL, WKS, RSR) appreciate support from the Institute for Basic Science (IBS-R019-D1).

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-352**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Wrinkle-free monolayer graphene grown on Ni(111) foils

Yongqiang Meng, Meihui Wang, Won Kyung Seong*, Rodney Ruoff[1,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea
[1]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

Chemical vapor deposition of carbon precursors on metal substrates (and most typically on copper foils) is now used for the scalable production of large-area, high-quality graphene films. However, as the metal foil cools from the (typically quite high) graphene growth temperature to room temperature, wrinkles (ripples or folds) occur due to the interfacial compressive stress caused by a relatively large thermal contraction of the metal foil. This thermal contraction and resulting compressive stress causes deadhesion in certain regions, even when there is epitaxy between a single crystal graphene film and a single crystal Cu(111) foil, for example. Controllable preparation of ‘wrinkle-free’ graphene is still challenging. And yet, we find ‘wrinkle-free’ monolayer graphene grown on Ni(111) at high temperatures. Scanning electron microscopy and atomic force microscopy are used to look into the morphology of these graphene films, which show no wrinkles. This study is “in progress” and the processes for, and the structure of, this ‘wrinkle-free’ graphene is now being studied further.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-353**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Multi-layer Layered Double Hydroxides on Aluminum Metal

Yongju Lee, Duk-Young Jung*

Department of Chemistry, Sungkyunkwan University, Korea

We synthesized layered double hydroxides (LDH) multilayers on aluminum metal substrates to understand the growth mechanisms of LDH and to prevent structural transformation of LDH in an aqueous solution. LiAl-LDH nanocrystals (NCs) were synthesized by oxidation of aluminum metal substrate in lithium salt solutions with urea, as supports to grow the secondary MgAl-LDH and LiAl-LDH NCs. The growth of LiAl-LDH NCs is strongly correlated with lithium salt types under supersaturation conditions. By applying the dissolution-reprecipitation mechanism, the secondary LDH NCs could be achieved on the amorphous Li-Al-O-OH of two shapes formed from calcination of LiAl-LDH NCs, demonstrating the surface morphology of the amorphous Li-Al-O-OH plays a crucial role to obtain large LDH crystals. We propose a new growth platform of the multilayers on the as-prepared LDH NCs depending on properties of surface, crystal structure, and types of salts under supersaturation conditions.

Poster Presentation : **MAT.P-354**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Selective capture of CO_2 under low pressure using metal-organic framework (MOF-808) functionalized with ethyleneamines

So Yeon Lee[*], **Sung Hwa Jhung**[1,*]

department of chemistry, Kyungpook National University, Korea

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

MOF-808 (a Zr-based metal-organic framework, MOF) was functionalized with ethyleneamines such as tetraethylenepentamine (TEPA), diethylenetriamine (DETA), and ethylenediamine (ED) to utilize the obtained MOFs in selective capture of CO_2 from offgas under low pressure. The modification was done firstly in the liquid phase via an acid-base reaction (using μ-OH of the MOF), and TEPA was the most effective among the tested ethyleneamines because of the low basicity of the TEPA. MOF-808s functionalized with TEPA were very efficient in CO_2 capture because of loaded primary and secondary amino groups. For example, one MOF-808, functionalized with an adequate quantity of TEPA, showed remarkable performances in CO_2 adsorption with a very high ideal adsorption solution theory selectivity of 256 which is around 7 times that of the pristine MOF-808. Moreover, the modified MOF-808 adsorbed around 2.5 times CO_2 that of the pristine M-808 at 15 kPa. The noticeable performance of the functionalized MOF-808 was explained with the loaded amino groups that are capable of a Lewis acid-base interaction with CO_2 to form carbamates. This work will pave the way to modify a MOF, although without open metal sites, to introduce amino groups that will be very effective in selective capturing of CO_2 from offgas.

Poster Presentation : **MAT.P-355**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

1. Modeling the structure of a Faujasite zeolite-templated carbon2. Exploring the Interface Chemistry of Hydrogenated Graphene on Cu(111): Insights into Covalent Cu-C Bonding

Alisher Fatkhulloev, **Madi Arsakay**[1,*], **Sun Hwa Lee**, **Won Kyung Seong**, **Rodney Ruoff**[2,*], **Maksim Rabchinskii**[3]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science, Korea*

[2]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

[3]*Center of Multidimentional Carbon Materials (CMCM), Institute for Basic Science, Korea*

1. We made a model of zeolite-templated carbon (ZTC) templated inside faujasite (FAU-type) zeolite pores with trivalently-bonded carbons forming the three-dimensional porous structures. This model provides insight into the two distinctive surfaces, and volumes, of our ZTC. Simulated X-ray diffraction patterns showed that a long-range structure order derived from zeolite (111) and (220) planes is still preserved even when 92% of the C atoms are removed from the neck regions and 23% from the super cage regions, also in reasonable agreement with experimental data. Our model clearly shows that the neck region (12 membered ring) of FAU, almost 7 Angstroms in diameter, cannot accommodate a completely formed, trivalently bonded carbon network—ever; there simply is no room. 2. The previous experimental work from our group (F-diamane, Nature Nanotechnology [1]) described chemically induced transformation of AB-stacked bilayer graphene into fluorinated single-layer diamond of essentially C 2 F stoichiometry with C(sp 3)-C(sp 3) interlayer bonding. Building on this we theorize that monolayer single crystal graphene which is epitaxial or close to epitaxial with Cu(111) surface that it is grown on, would develop Cu-C bonding due to hydrogenation of the open graphene surface. Our theoretical findings are supported by experimental data: valence band (VB) photoelectron spectroscopic measurements indicate the emergence of a set of electronic states corresponding to Cu-C bonding in the VB. Detailed

analysis of these interface bonds including Bader charge, electron density contours and C-Cu bond lengths will be reported at this KCS Meeting.

Poster Presentation : **MAT.P-356**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

On the interplay between chemistry, electronic structure, and optical properties of graphene derivatives: revisiting the puzzling complexity

Maksim Rabchinskii, Maria Brzhezinskaya[1], Seung Kyu Min[2], Rodney Ruoff[3,*]

Center of Multidimentional Carbon Materials (CMCM), Institute for Basic Science, Korea

[1]*BESSY II Facility, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany*

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

[3]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

Understanding how to tailor the band structure and optical properties of graphene-based materials through derivatization continues to be an intricate question owing to the puzzling interplay between the chemistry of graphene derivatives and their physical properties. Here, we provide a systematic study on the role of introduced functional groups and alterations in the π-conjugated system in determining the density of states (DOS) and optical absorbance in graphene. We have found the appearance of sets of localized states in the valence band (VB) of graphene which are related to molecular orbitals of the introduced functionalities. The interpretation of the origin of the arising states is made and their designation, pointing out their symmetry type, is proposed. Taking advantage of these results, we formulated and thus stated an empirical approach, allowing one to analyze and predict the impact of a certain functional group on the electronic structure of the functionalized graphene. Conversely, the absence of any substantial effect of oxygen-containing and other chromophore groups on the optical absorption in graphene derivatives, particularly graphene oxide has been clarified. We find that the optical absorption is governed solely by the extent and configuration of π-conjugated areas, revealing the appearance and evolution of a set of absorption bands in the near UV region upon alterations in the chemistry. We appreciate the support from the Institute for Basic Science (IBS-R019-D1).[1] Shnitov, V. V.; Rabchinskii, M. K.; Brzhezinskaya, M. et al. Small 2021, 17, 2104316.

Poster Presentation : **MAT.P-357**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Fluorination of carbon nanotubes with different diameters and chiral indices utilizing xenon difluoride

Yang Liu, Rodney Ruoff[1,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[1]*Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea*

Fluorination of carbon nanotubes (CNTs) has been reported rather extensively in the literature. I am participating in studies of fluorination of CNTs with a homebuilt system that uses xenon difluoride. We plan to fluorinate single-walled carbon nanotubes (SWCNTs) and double-walled carbon nanotubes (DWCNTs) with specific chiral index and diameter designated by the n and m indices. My research involves separating DWCNTs from one another that enables a more straightforward assignment of the (n1, m1), (n2, m2) indices of DWCNTs ("1" corresponds to the inner shell and "2" to the outer shell), where these indices can be measured by spectroscopy. This project has been underway for a few months. I am a visiting scholar at the Center for Multidimensional Carbon Materials (CMCM) from Sichuan University in China, where I am an associate research fellow. I look forward to meeting Korean and other chemists at this meeting! We appreciate support from the Institute for Basic Science (IBS-R019-D1).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-358**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Stimuli-responsive azo-based fluorophores and their alkyl length effect on fluorescence characteristics

Pyae Myat Phyo Thu, Mina Han[1,*], Sanghyuk Park[2]

Chemistry Department, Kongju National University, Myanmar

[1]*Department of Chemical Education, Kongju National University, Korea*

[2]*Department of Chemistry, Kongju National University, Korea*

As fluorescent stimuli-responsive materials are of great interest because of their wide applications in optoelectronic and biomedical systems, the fabrication of these materials in effective way had been developing. Here in, azobenzene-functionalized pyrene derivatives with different alkyl linkages: methoxy (AzMePy) and butoxy (AzBuPy) were synthesized and their photophysical and photochemical properties in N, N-dimethyl formamide (DMF) and DMF-H2O were investigated. Both compounds exhibited remarkable UV light responsiveness in solution (AzMePy: ~70% and AzBuPy: ~94%) which are observed from 1H NMR and UV-Vis absorption spectroscopy. The turbid suspension DMF-H2O of AzBuPy had notable photoisomerization, additionally the encapsulation and release of guest fluorophore, 9,10-diphenylanthracene (DPA), in AzBuPy was able to be stimulated by light and temperature respectively. Moreover, depending on the alkyl length, the two compounds showed distinct emission characteristics; the fluorescence spectra of AzBuPy presented only monomer emission, while AzMePy possessed dual monomer and excimer emission even in dilute solution which is probably influenced by the proximity of pyrene units. Furthermore, the concentration dependent self-assembled structures of AzMePy transformed from incomplete flakes to well-completed rectangular structures by varying the concentration of mixed solution, while AzBuPy showed flat petal like structures which can respond to non-invasive stimuli, light.Keywords: azo-based fluorophores, Photoisomerization, Excimer formation, Stimuli-responsive

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-359**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Preparation of ceramic/nickel composites using preceramic polymers and their use as HER catalyst

Young-Je Kwark[*], Sun-ung Moon[1]

Department of Materials Science Engineering, Soongsil University, Korea
[1]*Department of Green Chemistry and Materials Engineering, Soongsil University, Korea*

Ceramic materials have found extensive utility as support matrices for augmenting the catalytic efficacy of metallic catalysts. Nonetheless, the amalgamation of ceramics and metals entails intricacies arising from the imperative inclusion of supplementary agents such as binders. Moreover, achieving a uniform dispersion of catalysts within ceramic matrices presents a formidable challenge. Addressing these challenges, the current investigation employs preceramic polymers as precursor substances for ceramic fabrication. Through the composition of preceramic polymers with nickelocene, followed by uncomplicated pyrolysis, a novel class of ceramic/nickel composites is synthesized. These composites exhibit homogeneously dispersed nickel particles or nickel silicide at the nanometer scale. Characterization of the ensuing microstructure of these ceramic/nickel composites, synthesized across varying pyrolysis temperatures, is undertaken employing an array of analytical methodologies, including BET analysis, XRD, TEM, and ICP-AES. In addition, we evaluated the catalytic performance of these composites in hydrogen evolution reactions to investigate the effect of pyrolysis temperature.

Poster Presentation : **MAT.P-360**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Metal Nanocatalyst-Loaded Covalent Framework Membrane Nanoreactors: A Versatile Platform for Precise Catalytic Control, Enhanced Performance, and Long-Term Reusability

Dawoon Jeong, Ji-Woong Park[1,*]

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

We designed a versatile catalytic membrane nanoreactor via encapsulating metal nanocatalysts into bicontinuous nanopores, which presented an excellent catalytic performance in nanocatalysis.The nanoporous network materials were prepared from mixtures of poly(ethylene glycol) and the cross-linked polyurea-based organic network, followed by selective extraction of the polymer part. Then, a free-standing film of the network material was prepared by casting the mixtures onto the glass plate, followed by solvent evaporation.Due to the three-dimensional rigid pore continuity, the resulting membrane showed excellent chemical stability against organic solvents. In addition, the well-defined nanoporous channels permitted substances to enter/exist effectively via external convection and provide homogenous adsorption sites for metal nanocatalysts due to the metal precursor ion movement restriction.The reduction of metal precursor confined in a nanochannel with narrow pore size distribution proceeded in a diffusion-controlled manner, yielding ultrafine metal nanoparticles with an average diameter within 1~2 nm, in which the number density and dispersity of the particles could be adjusted by varying the reaction parameters involved in synthetic procedures.Taking advantage of the free-standing thin membrane supported into metal nanocatalysts within the nanoporous channel, they are a versatile catalytic nanoreactor platform that can be operated in both bath and continuous flow modes. In the batch mode, as-synthesized nanoreactors showed excellent catalytic conversion/reusability due to the facile quantification methods. Furthermore, a precise adjustment of reaction parameters in flow conditions allowed the continuous synthesis of fine chemicals with high selectivity.

Poster Presentation : **MAT.P-361**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Cobalt-Based Metal-Organic Framework for Photocatalytic Hydrogen Production: An Impact of Amino Functional Group

Yollada Inchongkol, Taya Saothayanun*, Sareeya Bureekaew*

Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Thailand, Thailand

An efficient hydrogen (H_2) production via photocatalytic water splitting was demonstrated using a cobalt-based metal-organic framework (MOF). The high H_2 production of about 25 mmol $gMOF^{-1}$ in 4 h can be achieved in the present fluorescence (FI) as a photosensitizer and triethylamine (TEA) as a sacrificial agent. Due to the framework's robustness, its structural integrity and catalytic reactivity remained unaffected even after the reaction. Furthermore, the impact of a substituent group ($-NH_2$) within the framework on catalytic performance was investigated.

Poster Presentation : **MAT.P-362**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Nanoarchitectural engineering of iron-doped layered titanium oxide with hollow structures for advanced sodium-ion battery

Seung-Min Paek[*], Gichan Kim

Department of Chemistry, Kyungpook National University, Korea

The recent expansion of the electric vehicle market has led to significant growth in demand for secondary batteries, particularly lithium-ion batteries (LIBs). However, the uneven distribution of lithium in the Earth's crust poses a sustainability challenge, leading to the development of various next-generation energy storage devices. In particular, sodium is abundant on Earth, making sodium-ion batteries (SIBs) a promising alternative. However, due to the large radius and slow kinetics of sodium ions, graphite-based anode materials used in conventional lithium-ion batteries cannot be utilized, and new anode materials must be developed. In this regard, attempts have been made to utilize titanium oxide (TiO_2) as an anode material for SIBs because of its structural safety, low cost, and environmental friendliness. However, existing TiO_2-based materials have low conductivity, which limits their electrochemical performance and requires improvement. This study presents a nanoarchitecture engineering strategy of iron-doped layered titanium oxide for high-performance sodium-ion battery applications. $Fe_{0.8}Ti_{1.2}O_4$ nanosheets (FTO NSs) were synthesized via a solid-state synthesis method using Fe_2O_3, K_2CO_3, and TiO_2 (anatase) and a series of ion exchange reactions. FTO NSs were controlled into hollow spheres utilizing the LBL self-assembly method, and XRD and HR-TEM confirmed the crystallographic structure of this process. The improved electrochemical performance of FTO-HS was compared to TiO_2-HS.

Poster Presentation : **MAT.P-363**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Enhanced UV-stability and efficiency of cobalt-triazole framework via Zn substitution for photocatalytic hydrogen production

Taya Saothayanun, Sareeya Bureekaew[1,*]

School of Energy Science and Technology, Vidyasirimedhi Institute of Science and Technology, Thailand
[1]*School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand*

Regulating metal at atomic levels into metal-organic frameworks (MOFs) plays important strategy to design high performance porous materials for diverse applications, in particular photocatalysis. Here, we reported a mixed-metal MOF composed of Co and Zn nodes and 1,2,4-triazole ligand as highly active and robust photocatalyst for H2 generation from aqueous triethanolamine solution without cocatalysts and sensitizers. Ligand-to-Metal charge transfer driven by UV light was observed for CoZn MOF. Advanced microscopic and spectroscopic analyses of CoZn MOF in bulk and local environments revealed homogeneous distribution of Zn and Co along the framework. The stability and photoactivity improvement of CoZn MOF over the monometallic isorecticular analogues were ascribed to the substituted Zn (fully filled d-orbitals) with electron-donating characteristics. The findings shed light on the potential of Co-triazole framework with as intrinsic photocatalyst and offer an effective route for its further development.

Poster Presentation : **MAT.P-364**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Ni-based Metal-Organic Framework as a Nanoreactor for an Enantioselective Production of Lactic Acid

Panyapat Ponchai, Kanyaporn Adpakpang, Sareeya Bureekaew*

Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Thailand

A highly durable Ni-triazolate framework endowing hydrophilic pores with spatial shape and size is employed as an efficient catalyst for the conversion of xylose to lactic acid (LA) under microwave radiation. The Ni-MOF catalyst can deliver a great yield of LA through C5-backbone cleavage and it excel in achieving high selectivity over furfural, a competitive cyclodehydration product. Interestingly, despite without typical chiral features of Ni-MOF, an enantiomeric excess (ee) of L-LA *c.a.* 58 % can be produced. The stereoselective production of LA over Ni-MOF is mainly ascribed to the special pore's architecture of Ni-MOF. This new finding highlights the unique features of MOFs catalyzing atypical reactions.

Poster Presentation : **MAT.P-365**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis and characterization of FeSe nanomaterials in a two-dimensional cluster configuration

Yujin Choi, Jaebeom Lee[1,*]

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

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

Renewed interest has been sparked in recent years regarding transition metal chalcogenides, owing to their distinctive properties and broad array of potential applications as nanomaterials. Among them, FeSe has garnered significant attention as a two-dimensional layered structure, with exceptional performance as both a superconductor and a thermoelectric material. Moreover, it presents a promising avenue for the development of next-generation electronic devices. In this research, we present our recent endeavors in exploring the optical and optoelectronic properties of FeSe nanoplates synthesized through hydrothermal methodologies. To comprehensively analyze the samples, a range of characterization techniques were employed, including power X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), and ultraviolet-visible (UV-Vis) spectroscopy. The creation of novel two-dimensional nanocrystals and the discovery of their extraordinary properties offer an effective pathway towards unraveling the intrinsic relation between conventional superconductivity and Mott physics states.

Poster Presentation : **MAT.P-366**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Nanoporous ZSM-5 Particles Coated with Silicalite-1 for Adsorption Ammonia in High Humid Environment

Lee Jea won, Ji Man Kim[1,*]

Sungkyunkwan University, Korea

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

Zeolites has been widely applied in industrial processes, such as catalysis, adsorption, separartion, and etc. Especially ZSM-5, can be used for Ammonia adsorption. However, in high humid environment, the competitive adsorption occur between water and ammonia because ZSM-5 which has SiO_2-Al_2O_3, can be related to the polarity of the adsorbed molecules. Additionally, silicalite-1 has only SiO_2 and possesses the MFI-type framework similar to ZSM-5 and, due to its characteristics, has a high silica content. As a result, such a zeolite is generally suitable for the adsorption of relatively non-polar substances. ZSM-5 coated with silicalite-1 can have selectivity between water and ammonia, also the thickness of the coated layer can be adjusted by secondary growth via hydrothermal synthesis.

Poster Presentation : **MAT.P-367**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Porous conductive cobalt-based metal-organic frameworks as promising electrocatalysts

Kanyaporn Adpakpang, Sareeya Bureekaew[*]

Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand

Metal-organic frameworks (MOFs) are a class of porous crystalline materials composed of metal nodes and organic linkers. MOFs are recognized as functional materials in various fields attributed by the rational designed properties. Electrocatalysis is one of the applications that MOFs are emerged since the frameworks can provide plenty of redox active catalytic (single)sites which can be accessible through their porous structures resulting in the excellent electrocatalytic activities. Enhanced catalytic performance such as reaction kinetics can be introduced via the intrinsic electrical conductivity of the MOF catalysts. In this work, Co-based MOFs constructed with azo ligand achieved by a simple microwave synthesis were studied for water electrolysis. Physicochemical and electrical properties attributed to electrocatalytic activities were investigated and discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-368**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Azobenzene-containing fluorescent compounds capable of photoisomerization with high efficiency

Mina Han[*], **Pyae Myat Phyo Thu**[1]

Department of Chemical Education, Kongju National University, Korea

[1]*Chemistry Department, Kongju National University, Korea*

We describe the synthesis of azobenzene-containing fluorescent compounds and their assembly into flat aggregates capable of repeated switching of their absorption and fluorescence characteristics in response to light and thermal treatment. The introduction of a relatively longer butyl linker between the pyrene and azobenzene (AzO4Py) resulted in the production of more than 90% of cis-form at the photostationary state of ultraviolet (UV) light, as determined absorption and 1H NMR spectral data. Flat micrometer-sized structures formed in polar DMF-H2O mixtures did not experience severe disassembly even after sufficient UV light irradiation, and showed excellent photoswitching performance. In addition, we examined the delivery functions of conventional hydrophobic fluorophores (9,10-diphenylanthracene: DPA) of DPA@AzO4Py aggregates obtained from the AzO4Py and DPA mixtures.

Poster Presentation : **MAT.P-369**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

A Novel Fluorophore based on Single Benzene for Hydrazine Visualization

Jisoo Kang, Dokyoung Kim[1,*]

Department of Biomedical Science, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Hydrazine (N_2H_4) is a crucial reagent utilized in various industries such as pharmaceuticals, aerospace, and agriculture due to its diverse applications. However, stringent regulations and careful handling are essential due to their potent toxicity when exposed to humans and animals. To mitigate hydrazine exposure, numerous detection methods have been established, with fluorescent-based approaches garnering particular attention for their efficacy and excellence, prompting extensive research.In this study, we disclosed a novel single benzene-based fluorophore (SBBF), HP that selectively reacts with hydrazine. Interacting the electron-donating and electron-withdrawing group within the single benzene unit, HP exhibits a large Stokes shift (172 nm) upon hydrazine interaction. This transition from blue to green fluorescence facilitates hydrazine detection in natural environments. We confirmed the capability of HP to detect hydrazine in diverse applications, including paper strips, soil, and three types of water samples. This research presents HP as an innovative hydrazine-specific fluorescent probe, poised to exert a positive impact across various domains.

Poster Presentation : **MAT.P-370**

Material Chemistry

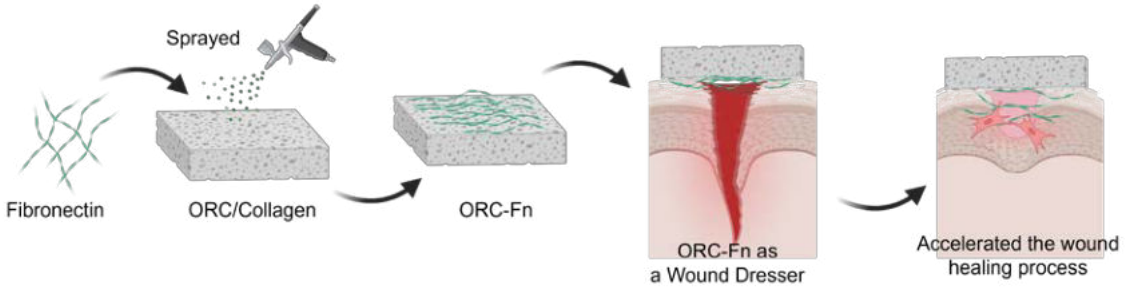
Exhibition Hall C FRI 11:00~13:00

Scalable Fibronectin-Coating Strategy for Wound Dressing Composites Using Spray Technique

Albertus Ivan Brilian, Sang Ho Lee, Kwanwoo Shin[*]

Department of Chemistry & Institute of Biological Interfaces, Sogang University, Korea

Fibronectin (FN), an adhesive glycoprotein, holds pivotal significance in wound healing, playing integral roles in extracellular matrix (ECM) formation and re-epithelialization. However, the effective integration of FN into wound dressings poses challenges due to the limitation of current chemical, mechanical, or extrusion-based methods. In this study, we explored the application of a spraying technique to coat FN onto the surface of commercially available oxidized regenerated cellulose (ORC)/collagen composites for the scalable production of FN-incorporated wound dressings. Our findings revealed that FN-coated ORC/collagen, achieved through spraying FN solution in DIW, exhibited superior shape retention compared to conventional manual methods like dropping or dipping. The successful deposition of FN was visualized via fluorescent conjugation, evident within both the micro-droplets and the ORC/collagen matrix. Intriguingly, the FN structure underwent unfolding upon spraying, as characterized using Fluorescence Resonance Energy Transfer (FRET). Additionally, in vitro assessments highlighted elevated cell viability within ORC/collagen-FN samples after 24 hours of incubation compared to pristine ORC/collagen. Collectively, our findings underscore the potential of the spraying technique for industrial-scale FN-coated wound dressing production, offering a promising avenue for enhancing wound healing outcomes.


Sprayed
Fibronectin
ORC/Collagen
ORC-Fn
ORC-Fn as
a Wound Dresser
Accelerated the wound
healing process

Poster Presentation : **MAT.P-371**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

ß-phase $M_xV_2O_5$ (M= Ca, Na) as New Viable Cathode Materials in Calcium-Ion Batteries

Richard Prabakar, **Myoungho Pyo**[1,*]

Department of Advanced Components and Materials Engineering, Sunchon National University, Korea

[1]*Department of Advanced Components and Materials Engineering, Suncheon National University, Korea*

Despite theoretical advantages, lack of reliable positive host materials capable of reversibly intercalating Ca^{2+} ions over extended cycles hinder the practical applications of calcium ion batteries (CIBs). The existing CIB cathode materials, to date, suffer severely from hysteric and capacitive voltage behavior, making them impractical. Herein, we describe and compare the performances of crystalline water-free ß-phase $Ca_{0.14}V_2O_5$ and $Na_{0.33}V_2O_5$, as new Ca^{2+} insertion electrode materials in CIBs in carbonate type electrolyte. The ß-phase materials deliver reversible capacities of ca. 247 and 180 mAh g^{-1}, respectively, corresponding to the insertion/extraction of Ca^{2+}. The sequential filling of Ca^{2+} in the three M1, M2, and M3 sites are verified in a ß-phase $Ca_{0.14}V_2O_5$. Initial insertion of Ca^{2+} causes a slight shift of oxygen atoms surrounding hepta-coordination sites, creating penta-coordinated sites that are then partially filled up to $Ca_{0.33}V_2O_5$. Further insertion occurs through stepwise occupation of up to 50% of neighboring hexa- and tetra-coordination sites to form $Ca_{0.67}V_2O_5$ and $Ca_{1.0}V_2O_5$, respectively. However, in a sodium counterpart the Na^+ preoccupied M1 sites ($Na_{0.33}V_2O_5$) direct the incoming ions in an unusual sequence, resulting in a 2 phase reversible Ca^{2+} insertion process. We attempt to understand and verify this contrasting Ca^{2+} insertion process and the accompanying structural relaxation via theoretical and experimental methods

Poster Presentation : **MAT.P-372**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Rhenium Redefined as Electrocatalyst for Hydrogen Evolution Reaction

Jinho Kim, Seok Min Yoon[1,*]

Department of chemistry, Wonkwang University, Korea

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

Rhenium-based catalysts has great potential for green hydrogen production via water electrolysis. Re's electrocatalytic activity for the hydrogen evolution reaction (HER) can be rival with platinum group metals (PGMs) theoretically, and Re is much more cost-effective than Pt. Despite the expected advantages of Re as a catalyst for HER, metallic-Re-based electrocatalysts have exhibited lower HER performances than PGMs-based catalysts experimentally. Herein, to improve Re's electrocatalytic activity, minuscule amount of Pt- and Ni (5 mol%) were doped to Re nanoparticle clusters interconnected by amorphous carbon (Pt-Ni@Re/C NPCs), which were superb than Pt/C. Pt-Ni@Re/C NPCs achieved phenomenally enhanced electrocatalytic HER performance in both acidic and alkaline media. Particularly in alkaline media, Pt-Ni@Re/C NPCs outperformed Pt/C or Pt-NiO/Ni with low overpotential (36 mV at 10 mA cm^{-2}), a Tafel slope (30 mV dec^{-1}), and excellent stability. The Faradaic efficiency for HER reached 98.63%. Pt-Ni@Re/C NPCs also possessed a low overpotential (419 mV) and high TOF value (195.6 s^{-1}) for vigorous evolution of hydrogen gas at a high current density (1000 mA cm^{-2}). Such high performance was corroborated by density functional theory studies. This design holds promise for advancing industrial green hydrogen production.

Poster Presentation : **MAT.P-373**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Atomically Dispersed Non-Precious Metal Catalysts for Electrochemical Chlorine Evolution Reaction

Jinjong Kim, Sang Hoon Joo*

Department of Chemistry, Seoul National University, Korea

Chlorine evolution reaction (CER) is an important anodic reaction in the chlor-alkali process. Dimensionally stable anode (DSA), precious metal oxides coated on a titanium electrode, has been extensively used as a CER catalyst during the past half-century. However, the DSA requires at least 30 at% of precious metals and catalyzes oxygen evolution reaction as a parasitic reaction, invoking the cost and selectivity issues, respectively. In this work, we have synthesized atomically dispersed non-precious metal (M; M = Fe, Co, Ni, and Cu)-based CER catalysts for unraveling their catalytic trends for the CER. The catalysts were synthesized by coating carbon nanotube (CNT) with a thin polyaniline layer (aniCNT), adsorption of a metal salt, overcoating of a silica layer, annealing at high temperatures, and etching of the silica layer. Among the resulting M_1/aniCNT catalysts, the Ni_1/aniCNT catalyst exhibited the best CER activity, which was superior to that of the DSA. In addition, all M_1/aniCNTs showed over 90% selectivity in similar conditions with the chlor-alkali process. The Ni_1/aniCNT catalyst may broaden the compositional range of CER catalysts, which has thus far been predominantly limited to precious metals.

Poster Presentation : **MAT.P-374**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

General Synthetic Method of Mesoporous Atomically Dispersed Nickel Catalysts for Electrocatalytic H2O2 Production

Sang Hoon Joo*, Jinjong Kim[1], June Sung Lim[2]

Department of Chemistry, Seoul National University, Korea

[1]*Seoul National University, Korea*

[2]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

Hydrogen peroxide (H_2O_2) is a key chemical that has found widespread utility in chemical industries, from disinfectants to semiconductor etchants. The electrosynthesis of H_2O_2 via oxygen reduction ($2e^-$ORR) has received increasing attention, as this method allows clean and sustainable on-site H_2O_2 production. Since the ORR can produce H_2O ($4e^-$ ORR) or H_2O_2 ($2e^-$ ORR) depending on the reaction pathways, it is crucial to develop electrocatalysts that can selectively produce H_2O_2. Drawing inspiration from the structure of metalloenzyme called superoxide dismutase (SOD) that catalyze superoxide ions ($O2\cdot^-$) into H_2O_2 and H_2O, we design high-performance Ni-based electrocatalysts for H_2O_2 production. We have prepared a series of mesoporous atomically dispersed Ni catalysts containing distorted square planar Ni^{2+}–N_x sites. Toward designing electrocatalysts with high H_2O_2 production activity and selectivity, we tuned the complexation between Ni cation and N-containing 1,10-phenanthrene by the judicious choice of a solvent, the ratio between Ni cation and phenanthrene, and the type of surface functional groups (N and O). The KSCN poisoning experiment revealed Ni^{2+}–N_x sites as active sites in the Ni–N/C catalysts. The optimized mesoporous Ni–N/C catalyst exhibited the best H_2O_2 electrosynthesis performance among the reported Ni-based atomically dispersed catalysts with a faradic efficiency of 86% and high stability over 24 h in alkaline conditions.

Poster Presentation : **MAT.P-375**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ca-doped Na_3ZnGaS_4 with improved ionic conductivity and stability for all-solid-state sodium-ion batteries

Jungyong Seo, Myoungho Pyo[*]

Department of Advanced Components and Materials Engineering, Sunchon National University, Korea

Na_3ZnGaS_4 is a new class of Na^+-conducting materials with a sturdy framework consisting of corner-shared super-tetrahedra. The ionic conductivity (σ_{ion}) of pristine Na_3ZnGaS_4 is quite low, but it can be improved by introducing defects. Herein, we describe the incorporation of vacancies into Na2 sites of Na_3ZnGaS_4 via Ca-doping ($Na_{3-2x}Ca_xZnGaS_4$; x = 0 ~ 0.2), which leads to a significant increase in σ_{ion}, reaching 0.28 mS cm^{-1} (hot-pressed $Na_{2.7}Ca_{0.15}ZnGaS_4$ pellet). The preferential residence of vacancies and Ca^{2+} in Na^+-conducting Na2 sites is theoretically and experimentally verified. Because of simultaneous location of vacancies and Ca^{2+} in Na2 sites, the increase in σion with 'x' in $Na_{3-2x}Ca_xZnGaS_4$ is not related to a decrease in the migration energy barrier (EA) but rather to an increase in effective hopping frequencies, compensating for the increase in EA. $Na_{2.7}Ca_{0.15}ZnGaS_4$ also exhibits excellent compatibility with Na_2Sn anode and TiS_2 cathode. A full cell (Na_2Sn | $Na_{2.7}Ca_{0.15}ZnGaS_4$ | TiS_2) delivers a discharge capacity of over 146 mAh g-1TiS_2 during 100 charge/discharge cycles at 0.12 mA cm^{-2} (120 mA $g^{-1}TiS_2$). In comparison to Na_3ZnGaS_4, $Na_{2.7}Ca_{0.15}ZnGaS_4$ also demonstrates inertness in various organic solvents, which is important for layer-by-layer stacking processes in the fabrication of all-solid-state batteries.

Poster Presentation : **MAT.P-376**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Defect Assessment of Boron Nitride Nanotube with Conjugated Polymer

Jeong-Seok Lee, Myung Jong Kim*

Department of Chemistry, Gachon University Global Campus, Korea

In this study, we examined the effectiveness of a self-assembly polymer-based method to assess the quality of boron nitride nanotubes (BNNTs) with varying diameters. BNNTs, known for their exceptional mechanical, thermal, radiation shielding, and insulating properties, hold immense promise for diverse applications. However, the lack of a universally accepted quality assessment method for BNNTs presents significant limitations in their study and practical utilization. There was a report that rra-P3HT makes distinctive spectroscopic changes when combined with BNNTs via π-π interactions. We tested different BNNT samples with varying diameters, and confirmed a correlation: increasing BNNT diameter reduces the intensity of spectroscopic changes. This insight guides future research in BNNT characterization and applications.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-377**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Understanding Surface Passivation of Silver Bismuth Sulfide Nanocrystals by Organic and Inorganic Ligands

Cheong Beom Lee, Hyosung Choi*

Department of Chemistry, Hanyang University, Korea

Silver bismuth sulfide nanocrystals (AgBiS2 NCs) have attracted significant attention as eco-friendly alternatives to toxic lead-based semiconductor materials. However, the photovoltaic efficiency of this material still lags behind that of lead-based materials, and the passivation of nanocrystal could enhance photovoltaic performance by preventing degradation. In this study, density functional theory (DFT) calculations were used to investigate the surface passivation of AgBiS2 by adsorption of organic ligands (ethanedithiol (EDT), malonic acid (MA), and mercaptopropionic acid (MPA)) as well as inorganic ligands (silver bromide (AgBr2) and silver iodide (AgI2)). For organic ligands, MPA had stronger adsorption strength compared to EDT and MA. For inorganic ligands, AgBr2 exhibited stronger adsorption compared to AgI2, resulting in effective surface passivation of AgBiS2 NCs. These results are also confirmed by experiments. Thus, our theoretical approaches might be useful to design highly active and stable photovoltaic device.

Poster Presentation : **MAT.P-378**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Reversible calcium ion electrodeposition with a dual additive system

Hyungjin Lee, Seung-Tae Hong[1,*]

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

[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Although, rechargeable lithium-ion batteries (LIBs) are widely employed for energy storage, necessitating advancements beyond current chemistry. Additionally, high costs, safety concerns, and limited lithium resources have led researchers to explore the multivalent ion batteries (e.g., Zn^{2+}, Al^{3+}, Mg^{2+}, and Ca^{2+}). Among them, Calcium ion batteries (CIBs) offer advantages. First, cost-effective due to its abundance. Second, effortless diffusion arisen from lower charge density (0.49) than other ions (e.g., Zn^{2+}(1.18), Mg^{2+}(1.28), and Al^{3+}(4.55 e/Å3)). Third, lower redox potential (-2.87 V vs SHE) compared to other ions (Mg: -2.37, Na: -2.71, K: -2.93, Li: -3.05 V vs SHE). Nevertheless, the absence of an electrolyte system that can be utilized for both cathode and anode simultaneously has resulted in the unavailability of Ca ion-full cell. Especially, the components of SEI layer which is formed by decomposition of electrolyte are Ca ion insulator. Hence, developing a suitable electrolyte system is crucial for the formation of the SEI layer on calcium metal, which should consist of stable compounds that facilitate the conduction of calcium ions. Here, we applied dual additive system for reversible Ca ion stripping and plating. Compared to pristine electrolyte or mono additive, the dual additive showed lower overpotential and high coulombic efficiency in cyclic voltammetry. Also, the plating of calcium was available up to 0.5 mAh/cm^2. According to linear sweep voltammetry, dual additive electrolyte was stable over 4 V (vs. Ca/Ca^{2+}). The plating of calcium was proved by X-ray diffraction(XRD) of current collector. Although the coordination environment of Ca-ion in dual additive system should be solved, it demonstrates the possibility of Ca full cell configuration with high energy density at room temperature.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-379**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Investigation of Calcium-ion Insertion and Extraction Mechanism in Manganese Niobium Phosphate as a New Cathode Material for Rechargeable Calcium-ion Batteries

Dongmin Lee, Seung-Tae Hong[1,*]

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

[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Compared to lithium-ion batteries, calcium-ion batteries offer several advantages such as high theoretical capacity due to the high electric charge of calcium-ions, low price due to their abundance, and safety. However, there is currently no suitable cathode material available for calcium-ion batteries. Recently, transition metal phosphates with a NASICON structure have been identified as a promising option. In this study, we introduce manganese niobium phosphate as a cathode material for a calcium-ion battery that was synthesized using a solid-state method. The crystal structure was analyzed by X-ray diffraction measurement and the element ratio of the material was analyzed by energy dispersive spectroscopy measurement, confirming successful synthesis. To measure the electrochemical performance of the material as a calcium-ion battery, various tests such as cyclic voltammetry, galvanostatic discharge-charge, X-ray diffraction, and elemental analysis were conducted. The electrochemical experiment revealed an initial discharge capacity of 120 $mAhg^{-1}$. After X-ray diffraction and elemental analysis, it was confirmed that calcium ions were successfully inserted and extracted reversibly into the material during the charging and discharging process. Overall, this study demonstrates the discovery of a promising new host material for calcium-ion batteries.

Poster Presentation : **MAT.P-380**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Crystal Water-free Iron Hexacyanoferrate: Preparation and Electrochemical Investigation as a Host Material for Calcium-ion Batteries

Jin Choi, Seung-Tae Hong[1,*]

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

[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Next-generation batteries are in high demand because lithium-ion batteries (LIBs) have a limited theoretical energy density. Among the potential successors to LIBs, calcium-ion batteries (CIBs) stand out due to their cost-effectiveness, abundance, and low redox potential. However, only a small number of materials have the ability to intercalate Ca^{2+} ions in a reversible and efficient way with a high energy density.Despite its recognition as a prospective cathode material due to its high theoretical energy density, iron hexacyanoferrate requires deeper investigation, particularly regarding the influence of crystal water content and its electrochemical characteristics. In our current study, we effectively produced a cubic-structured iron hexacyanoferrate without crystal water and extensively assessed it as an appropriate host material for CIBs. Confirmation of the absence of crystal water in the structure has been achieved through X-ray diffraction (XRD) and thermogravimetric analysis (TGA). Through galvanostatic electrochemical test, we observed an initial discharge capacity of 135 mAh g^{-1} at 20 mA g^{-1} and 128 mAh g^{-1} after 5 cycles. XRD and diverse elemental analyses were employed to confirm the reversibility of Ca^{2+} intercalation into the material. Ultimately, our findings offer significant insights into improving new host materials for CIBs with a substantial energy density.

Poster Presentation : **MAT.P-381**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Melamine phytate as an anti-termite agent

Sung Hyun Oh, Sanha Park, Jinkwon Kim*, Seog Woo Rhee*

Department of Chemistry, Kongju National University, Korea

In this study, a technique to treat pine (*Pinus densiflora*) blocks with melamine phytate and a method for effectively preventing termite access was investigated. The wood block was sequentially immersed in the melamine aqueous solution and the phytic acid aqueous solution so that solid melamine phytate was formed inside and on the surface of the wood block. Subterranean termites (*Reticulitermes speratus*) prevention experiments were carried out in choice and no-choice tests according to AWPA standard (E1-17). In the no-choice test, the termites did not eat the treated wood block at all, and all died between 19 and 22 days, indicating a 100% mortality. In the choice test performed for 28 days, termites ate little of the treated blocks and only ate untreated wooden blocks, and showed a slightly higher mortality (~26%) than that of the control group (~15%). In conclusion, melamine phytate showed performance as a very effective anti-termite agent.

Poster Presentation : **MAT.P-382**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Improving the ion conductivity by aliovalent-doping into Na halide solid electrolyte

Hyojin Kim, Hyungjin Lee[1], Seung-Tae Hong[2,*]

Department of energy science and engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

[2]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

The rapid growth of the lithium-ion batteries (LIBs) market is accompanied by persistent concerns regarding battery safety. In response to this challenge, our research has focused on the advancement of solid-state battery technology based on new solid electrolyte (SE) materials. Among solid state electrolyte candidates, halide SEs offer high stability window and sinter ability advantages, making them viable for all-solid-state batteries. Furthermore, due to the increasing cost of LIBs, various alternative ions are being proposed to address this problem. Among them, sodium ions are the most prominent candidates. Therefore, we conducted research on halide solid electrolytes based on sodium, considering it as a strong candidate instead of lithium. We synthesized of halide-based solid electrolyte through aliovalent doping into the Na-Zr-Cl composition. The effectiveness of the substitution within the Na-Zr-Cl composition was confirmed through X-ray diffraction (XRD) analysis by using Rietveld refinement techniques. Electrochemical Impedance Spectroscopy (EIS) was utilized to check the enhanced ionic conductivity of the sample in comparison to the pristine sample. Remarkably low electronic conductivity value was obtained, understanding its potential as a proper all-solid-state battery electrolyte. Through Linear Sweep Voltammetry (LSV), we confirmed the electrolyte's stability, with no decomposition even at voltages exceeding 3V (vs. Li/Li+). Additionally, the particle size distribution of the synthesized sample and the

uniformity of doping metal substitution were examined by SEM image with element mapping. Although the Na+ conductivity improved compared to the pristine, it was still insufficient for commercialization. Thus, the additional studies are needed to enhance the ionic conductivity of halide solid electrolyte discovering additional aliovalent or isovalent substitutions.

Poster Presentation : **MAT.P-383**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Investigating Novel Inorganic Solid Electrolytes, Lithium Indium Sulfide, for All-solid-state Batteries

Hyeonjin Seo, Seung-Tae Hong[1,*]

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

[1] *Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

This study investigates the use of inorganic solid electrolytes (SEs) in all solid-state batteries due to their superior thermal stability compared to organic liquid electrolytes. While sulfide SEs exhibit strong conductivity and easy sintering, they are susceptible to chemical instability and toxic gas release in moist conditions. Balancing conductivity, chemical resilience, and electrochemical stability in SE compositions presents a challenge. The study emphasizes the importance of exploring new SEs with diverse compositions and crystal structures.Notably, this research uncovers a disordered lithium and central metal structure in Li-M4+-S materials, alongside the emergence of a distinct trigonal arrangement upon M3+ ion substitution. The analysis extends to investigating the solubility limit of In3+, involving the substitution of In3+ for previously identified Al3+ and Ga3+ ions. Analytical techniques, including electrochemical impedance spectroscopy (EIS), X-ray diffraction (XRD) with Rietveld refinement, and Bond valence site energy (BVS) calculations, offer insights into material properties.Significantly, the study demonstrates enhanced conductivity(~10-5 Scm-1) in the new material, surpassing established Li-M4+-S materials(~10-7 Scm-1). Future research will evaluate In3+'s impact on air stability, alongside forthcoming assessments of cell capacity through cyclability and galvanostatic charge-discharge tests using a sulfide-based cathode.In summary, this study underscores the potential of the newly devised ion conductor to advance all-solid-state battery technology.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-384**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Sodium ionic conductors with new type of crystal structure

<u>Jihun Roh</u>, Hyojin Kim[1], Seung-Tae Hong[2,*]

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*

[2]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Sodium ion batteries (SIBs) are promising energy storage systems due to the abundant reserves and cost-effectiveness of sodium resources. Recent advancements in SIB technology have led to the emergence of solid-state batteries incorporating solid-state electrolytes (SSEs), enhancing their safety profile. In this study, we present two crystal structure of sodium ionic conductors, sodium thio-silicate. The two different polymorphs of new sodium thio-silicate were determined by powder X-ray diffraction for the first time. The high-temperature polymorph (HT-NSS) crystallizes in the tetragonal space group of $P4_2/mcm$ (No. 132) with lattice parameters a = 6.97153(15) Å, c = 12.0341(3) Å, and V = 584.88(3). The low-temperature polymorph (LT-NSS) crystallizes in the monoclinic space group of $P2_1/c$ (No. 14) with lattice parameters a = 6.7993(3), b = 14.3142(6), c = 17.4666(9), β = 112.145(2), and V = 1574.56(14). The main structure motif of HT-NSS shows isolated Si_2S_6 units of two edge-shared SiS_4 tetrahedra, while the LT-NSS shows isolated Si_3S_9 units of three corner-shared SiS_4 tetrahedra, with certain sulfur positions are vulnerable to oxygen substitution. The material displayed ionic conductivities of 1.85×10^{-7} S cm^{-1} at 303 K for HT-NSS, and 7.67×10^{-8} S cm^{-1} at 303 K for LT-NSS. Bond valence energy landscape (BVEL) calculation revealed three-dimensional sodium ion diffusion pathways, and activation energy of 0.393 eV and 0.421 eV in the unit cell. Our findings provide valuable insights for the design of novel ionic conductors tailored for all-solid-state battery applications.

Poster Presentation : **MAT.P-385**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Precise Pore Size Matching of Carbon Electrode with Redox Species for Improvement of Redox-Enhanced Electrochemical Capacitor Performance

Young Hun Cho, **Seung Joon Yoo***

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

Compared to traditional electric double-layer capacitors, aqueous redox-enhanced electrochemical capacitors (redox ECs) exhibit higher energy density and steadier power output due to the utilization of redox-active electrolytes. In this system, the interaction at the electrode/electrolyte interface, in addition to the solubility of redox materials, plays a pivotal role in the performance. Here, unlike common approaches involving electrode engineering (e.g., adjusting the carbon pore size), we explore a synthetic approache to optimize the electrode/electrolyte interaction by modifying viologen substituents to precisely match their size with the electrode pores. Through the performance analysis based on changes in the viologen substituent, we identified butyl viologen (BV) as the optimal choice for commercial activated carbon (MSC 30) due to its suitability at the electrode/electrolyte interface. The full cell using a 1 M BV/3 M NaBr electrolyte demonstrated remarkable outcomes: an energy density of 82.3 Wh/kg at 0.5 A/g, a power density of 5057 W/kg at 10 A/g, and stable energy retention of 95.34% after 10,000 cycles at 5 A/g. These results emphasize the potential of substituent-driven size tuning of organic redox materials as an effective method for tailoring the electrode/electrolyte interface in redox ECs. This study highlights the importance of precise size matching between electrodes and electrolytes in the design of high-performance supercapacitors.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-386**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Stable and High-Energy Zinc-Iodine Battery through Deep Eutectic Solvents (DES)

Jae Hyung Kim, Seung Joon Yoo[1,*]

MATERIALS SCIENCE AND ENGINEERING, Gwangju Institute of Science and Technology, Korea

[1]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

Aqueous zinc-iodine batteries are promising energy storage systems due to their cost-effectiveness and safety. Nevertheless, there exist challenges preventing the practical commercial utilization of zinc-iodine batteries, including dendrite growth, adverse side reactions, and limited operation in low temperatures. To address these challenges, researchers have explored zinc batteries with deep eutectic solvents (DES) containing hydrogen bond donors and acceptors. DES can mitigate side reactions and freezing point issues, yet they suffer from high viscosity and low conductivity. In this work, we introduce a new quaternary DES system based on, combining ZnCl2, sulfolane, water, and KI.In this multi-component system, ZnCl2 serves as a redox-active source, providing zinc and chlorine species. The robust interaction between sulfolane and water effectively suppresses undesired side reactions. Water's role as a hydrogen donor and acceptor promotes the creation of a deep eutectic solvent (DES). Consequently, addition of water leads to decreased electrolyte viscosity and increased ionic conductivity within the system. The resultant quaternary DES-based zinc-iodine battery demonstrates outstanding operational stability in a Zn//Zn symmetric test, exhibiting a remarkable 2700-hour stability under a current density of 2 mA/cm² ,2 mAh/cm². Additionally, in a full-cell configuration, the battery demonstrates a capacity limit of 250 mAh/g at a current density of 1 A/g. Impressively, the system also exhibits notable high-rate capabilities at 5 A/g (corresponding to 200 mAh/g). This system exhibits superior performance compared to other alternative zinc-iodine-based systems.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-387**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Methylene blue loaded-GNR@mSiO_2 core@shell nanocomposites integrated on graphene oxide; a multifunctional photo-nanotheranostic solution for cancer

Seohyeong Lee, Eue-Soon Jang[*]

Department of Applied Chemistry, Kumoh National Institute of Technology, Korea

Photo-nanotheranostics integrates diagnostics and therapeutics, triggered by near-infrared (NIR) light, into a singular phototheranostic nanomaterial. This innovation holds immense potential for early cancer detection and precise cancer treatment. This research introduces a comprehensive approach by creating methylene blue-loaded mesoporous silica-coated gold nanorods on graphene oxide (MB-GNR@mSiO_2 -GO) as an all-in-one photo-nanotheranostic agent. This agent enables intracellular surface-enhanced Raman scattering (SERS) imaging-guided photothermal therapy (PTT) and photodynamic therapy (PDT) for cancer treatment. The integration of MB-GNR@mSiO_2 onto GO nanosheets demonstrates uniform anchoring, yielding a remarkable photothermal conversion efficiency of 48.93%. This efficiency translates to exceptional PTT/PDT outcomes for cancer treatment. In vitro experiments reveal that laser-irradiated MB-GNR@mSiO_2 -GO substantially reduces cell viability (by 7.92%), resulting in comprehensive cellular destruction. Laser irradiation of MB-GNR@mSiO_2 -GO generates a robust SERS effect, indicating heightened SERS peaks for early cancer detection. This underscores the nanomaterial's potential for precise SERS imaging-guided synergistic PTT/PDT of cancer. Overall, MB-GNR@mSiO_2 -GO showcases significant promise for accurate, synergistic cancer treatment, guided by SERS imaging

Poster Presentation : **MAT.P-388**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Micro-needle photothermal patch system for improving wrinkles

Jiwon Choi, Eue-Soon Jang*

Department of Applied Chemistry, Kumoh National Institute of Technology, Korea

Micro-needles offer the advantage of painless direct delivery of macromolecular drugs into the epidermis, by passing metabolic degradation, and avoiding drug loss. However, drawbacks include the risk of infection due to bleeding and significant medical barriers, making commercialization challenging. To address these issues, micro-needles utilizing biocompatible polymers have been developed, with a length below 500μm to penetrate only the avascular epidermal layers, mainly for cosmetic purposes. However, these micro-needles face a drawback in the slow diffusion of wrinkle-improving active ingredients through the stratum corneum, primarily due to binding proteins in the dermal layer. In this study, we developed micro-needle and hydrogel photothermal patches containing gold nanorods with excellent photothermal effects at near-infrared wavelengths. Additionally, we designed a dedicated near-infrared light source to induce photothermal effects of photothermal patches. Clinical trial results revealed that micro-needle photothermal patch system exhibited a twofold improvement around the eyes compared to using of only micro-needle patch. This micro-needle photothermal patch technology holds the potential to provide a convenient transdermal drug delivery system for homecare, especially beneficial for patients in need of regular drug administration.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-389**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Formulation of Cosmetic Composites Incorporating Gold Nanorods for Infrared-A Radiation

Juhui Seo, Eue-Soon Jang*

Department of Applied Chemistry, Kumoh National Institute of Technology, Korea

Utilizing Gold Nanorods (GNRs) holds great potential in mitigating the effects of Infrared-A radiation (IR-A) due to their strong absorption within the IR-A wavelength range (λ= 700-1,400 nm) and biocompatibility. These attributes position GNRs as appealing candidates for advancing skincare products and protective solutions aimed at counteracting IR-A radiation-triggered skin aging and damage. This investigation delves into the efficacy of GNR composites with varying aspect ratios in blocking IR-A radiation. To increase IR-A blocking efficacy, we combined GNRs with scattering materials such as TiO_2 and ZnO nanoplates possessing high refractive indices within the IR-A spectrum. The impact of this IR-A blocking agent on human fibroblast cells was assessed, encompassing assessments of cell viability, Matrix Metalloproteinase-1 (MMP-1) expression, and generation of reactive oxygen species (ROS), juxtaposed with a control group exposed to IR-A radiation sans the blocking agent. Furthermore, clinical trials were conducted to validate the tangible effectiveness of the developed IR-A blocking agent.

Poster Presentation : **MAT.P-390**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Electrolytic Cancer Ablation Therapy Using Gold Nanorods as Electric Antenna

Yeong-Jun Jeon, Eue-Soon Jang[1,*]

Applied Chemistry, Kumoh National Institute of Technology, Korea

[1]*Department of Applied Chemistry, Kumoh National Institute of Technology, Korea*

Electrolytic ablation (EA) is an emerging new therapeutic technique that destroys solid tumors electrochemically that are clinically used in many counties. However, the clinical use of EA in treating diverse tumor types have hindered by limited effective areas and complicated electrode design. EA combining nanotechnology is urgently required for enhancing electrolytic tumor ablation therapy. Herein, we designed and proposed a new conceptual approach based on difructose dianhydrides IV conjugated polyethylenimine-polyethylene glycol-modified gold nanorods (DFA IV-PEI-PEG-GNRs) as electric nanoantennas and nano-electrocatalysts for electrolytic tumor ablation therapy. More interestingly, the square wave direct current (DC) electric field (EF) triggers an electrochemical reaction between water molecules and chloride (Cl) ions on the surface of GNRs (DFA IV-PEI-PEG-GNRs), generating major electrolysis reaction products such as hydrogen (H_2), oxygen (O_2) and chlorine (Cl_2) gases around the electrodes and resulting in significant pH changes that could induce cell death. In consequence, the DFA IV-PEI-PEG-GNRs show a significant curative effect in the treatment of solid tumors with large initial sizes (~ 300 mm^3) both in vitro and in vivo after DC electric treatments. The overall findings suggest that electrolytic tumor ablation therapy using DFA IV-PEI-PEG-GNRs offers a very promising avenue for more effective tumor treatment in the future.

Poster Presentation : **MAT.P-391**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Effect of Gallium on Silver Indium Gallium Sulfide Nanocrystals Photoluminescence

Jiyeon Ban, Haemin Song, Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

Alteration with heavy metal-free colloidal nanocrystals (NCs) has been extensively explored as an alternative to Cd-based CQDs. However, due to internal or surface defects, these Cd-free CQDs have shown unfavorable full width half maximum (FWHM) photoluminescence (PL). Here, we report non-stoichiometric $AgIn_xGa_{1-x}S_2$ (AIGS) NCs that exhibited blue-shifted PL with narrow FWHM as the synthesis temperature increased. The PL of the synthesized NCs reached an FWHM of 33.8 nm at 551.8nm. Through X-ray photoelectron spectroscopy studies, it has been demonstrated that the changes in the gallium oxidation state directly affect the blue-shifted narrow bandgap PL. In spite of narrow bandgap emission, the PLQY remains very low. ZnS shell on the AIGS NCs by successive ionic layer adsorption and reaction (SILAR) method lead to an improvement in the photoluminescence quantum yield (PLQY) up to 20%, and we successfully fabricate light-emitting-diode device as using AIGS/ZnS NCs. The External Quantum Efficiency (EQE) was 0.1%. These simply tunable optical properties and promising device application will give opportunities for Cd-free QDs applications.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-392**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Electrical behaviors of oxynitride perovskites $\mathbf{SrAl_{0.2}}\boldsymbol{M}_{\mathbf{0.8}}\mathbf{O_{2.4}N_{0.6}}$ ($\boldsymbol{M}$ = Nb, Ta)

Yang Hun Kim, **Young-il Kim**[1,*]

Department of Chemistry, Yeungnam university, Korea

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

Perovskite oxynitrides $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ (M = Nb, Ta) (M = Nb, Ta) were characterized by ac impedance spectroscopy (4 Hz ~ 8 MHz) using polycrystalline compacts with relative densities of 41 and 48 %. The equivalent circuit analysis of the Nyquist plots revealed that $SrAl_{0.2}Nb_{0.8}O_{2.4}N_{0.6}$ has dielectric constants (κ) as high as 1600~5000 in the temperature range, 250—350 K. On the other hand, the $SrAl_{0.2}Ta_{0.8}O_{2.4}N_{0.6}$ showed a markedly distinct dielectric behavior, with $\kappa \fallingdotseq 25$. The above contrast is attributed to the difference in polarizability of Nb and Ta. With increasing the temperature, the dielectric relaxation time decreased in $SrAl_{0.2}Nb_{0.8}O_{2.4}N_{0.6}$, and increased in $SrAl_{0.2}Ta_{0.8}O_{2.4}N_{0.6}$. In terms of electrical conductivity (σ), $SrAl_{0.2}Nb_{0.8}O_{2.4}N_{0.6}$ exhibited a typical semiconductor-type behavior from the bulk component: $\sigma = 1.68 \times 10^{-6}$ S cm^{-1} at 290 K, and an activation energy of 0.19 eV. Meanwhile, $SrAl_{0.2}Ta_{0.8}O_{2.4}N_{0.6}$ exhibited an unusual PTC (positive temperature coefficient of resistance) behavior.

Poster Presentation : **MAT.P-393**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Controlling Interband and Intraband Transitions in Silver Selenide Quantum Dots via Trioctylphosphine-Assisted Cation Exchange

Hyeong Seok Kang, Kwang Seob Jeong[1,*]

chemistry, Korea University, Korea

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

Cation exchange (CE) offers a method to obtain nanocrystals with compositions that are difficult to access using conventional synthetic approaches. CdSe colloidal quantum dots (CQDs) were successfully transformed into self-doped Ag_2Se CQDs exhibiting steady-state intraband transitions in the mid-wavelength infrared (MWIR) range using a silver precursor containing an excess of Ag^+. Tertiary phosphines such as tri-n-octylphosphine (TOP) can strongly interact with Ag^+ cations, thereby suppressing CE reactions and limiting the infiltration of Ag^+ cations into the nanocrystal interior. Here, we present a CE method utilizing TOP to control the Fermi level of product Ag_2Se CQDs. As the volume of TOP in the silver precursor increases, the Ag ratio in the product Ag_2Se decreases, leading to a decrease in the intensity of intraband transitions. This phenomenon suggests that a decrease in the Ag ratio composing the nanocrystals results in a reduction of the Fermi level. Experimental observations were conducted under various TOP volume conditions, revealing the transformation from CdSe CQDs to Ag_2Se CQDs and further to self-doped Ag_2Se CQDs, which were analyzed for their structural and optical properties using Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD), and transmission electron microscopy (TEM).

Poster Presentation : **MAT.P-394**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Facile synthesis method of self-doped mid-infrared Ag_2Se colloidal quantum dots

Ngoc Mai An, Jin Hyeok Lee[1], So Young Eom[1], Haemin Song[1], Kwang Seob Jeong[1,*], Minhaeng Cho[1]

Department of Chemistry, Center for Molecular Spectroscopy and Dynamics, IBS, Korea

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

Mid-infrared (IR) colloidal quantum dots (CQDs) have attracted significant attention due to their optical and electrical features that can be used for various thermoelectricity and infrared optoelectronic applications. Recently, non-toxic self-doped Ag_2Se CQDs were explored as a promising candidate for mid-IR photodetectors showing steady-state intraband transition (occurs in $1S_e$-$1P_e$ energy states between conduction bands). Comparable to the previously reported hot-injection and cation-exchange methods, we report a facile synthesis method of the self-doped Ag_xSe ($x>2$). This method has advantages in reducing the cost of material synthesis and enables widespread use of the self-doped non-toxic CQDs in various environments and applications. The result of crystal structure, compositional analysis, mid-IR absorption-photoluminescence, and mid-IR photocurrent response of as-synthesized Ag_xSe CQDs reveal the peculiar optical and electrical properties of the self-doped CQDs and potential as an IR active material for mid-IR-based optoelectronics.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-395**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Inclusion of kojic acid into the gallery of layered yttrium hydroxide and its tyrosinase inhibition behavior

Myeongjin Kang, Song-ho Byeon[1,*]

Applied Chemistry, Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Kojic acid (5-hydroxy-2-(hydroxymethyl)-4-pyrone) inhibiting the formation of dihydroxyphenylalanine from tyrosine in the process of melanin biosynthesis is useful to prevent oxidative browning of on cut fruits, preserve pink and red colors of seafood, and lighten skin in cosmetics. It has also antibacterial and antifungal properties. However, it is known that kojic acid is highly sensitive to sunlight, temperature, and oxygen. Its degradation products containing the 4-pyrone may have adverse effect on human health like benzene to cause serious side effects such as hepatocellular and thyroid adenomas. Therefore, it is required to find ways in avoiding direct contact with the skin and preventing them from degradation to maximize their efficiency. In this work, the kojic acid was intercalated into the layered yttrium hydroxide (LYH) via anion-exchange reaction in the interlayer space. Compared to free kojic acid, its stabilities against UV, heat, and oxygen were highly improved in the resulting KA-LYH, indicating effective confinement and protection from the attack of atmospheric oxygen in the gallery of LYH host. Nevertheless, the inhibition ability of tyrosinase was practically maintained through its release from the gallery of LYH in phosphate buffer solutions. The inclusion and release behaviors as well as the stabilities against heat, sunlight, and oxidation were systematically investigated to assess the tyrosinase inhibition of kojic acid in the interlayer space of LYH.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-396**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

A comparison study of MnO_2 cathodes for aqueous zinc-ion batteries

Nahyun Kim, **Chung-Yul Yoo**[*]

Department of Chemistry, Mokpo National University, Korea

Currently, the most commercialized lithium-ion batteries (LIBs) cannot meet the growing demand because it has limited lithium reserves. Accordingly, the development of alternative next-generation ion batteries is required. Recently, aqueous zinc-ion batteries (AZIBs) have been considered as an alternative system due to the low price of zinc and higher valency of zinc ions (Zn^{2+}). However, it is necessary to develop novel cathode materials in order to achieve high capacity and reversibility. In this work, we prepared three different types of MnO_2: amorphous α-MnO_2, crystalline α-MnO_2, and layered MnO_2 for the cathode materials for AZIBs. The electrochemical properties of these MnO_2 cathode have been systematically investigated by cyclic voltammetry, galvanostatic charge-discharge measurements, and ex-situ X-ray diffraction experiments. The impact of crystallinity and the structure of MnO_2 on the electrochemical intercalation/deintercalation of Zn^{2+} was discussed in detail

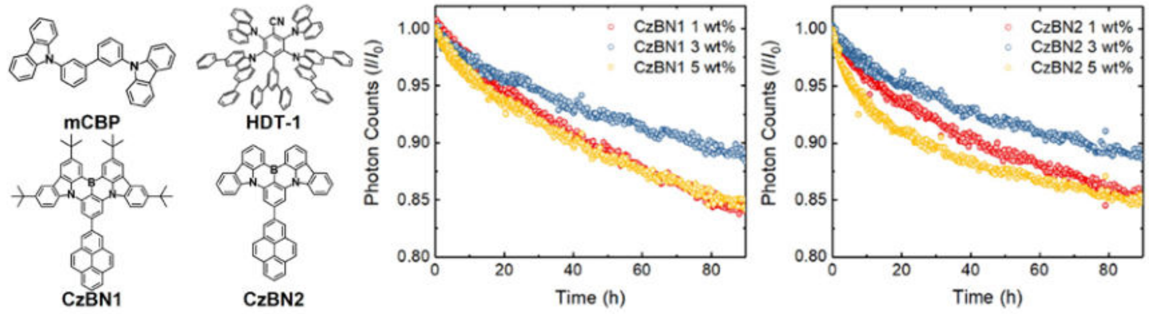
Poster Presentation : **MAT.P-397**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Investigation the Effect of Functional Groups on Hyperfluorescence Organic Light-Emitting Diodes with Multiple Resonance Terminal Emitter

Minho Jang, Chaewon Park, Sae Youn Lee[1,*]

Advanced Battery Convergence Engineering, Dongguk University, Korea
[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Organic light-emitting diodes (OLEDs) have been significantly improved and concerned as promising display technology due to better quality and wider applications. Accordingly, research regarding OLEDs has been focused to elucidate enhance excitation and emission mechanisms enabled by wide availability of organic materials.[1,2] Hyperfluorescence (HF) system that lights by integrating assistant dopant (AD) and terminal emitter (TE) with thermally activated delayed fluorescence (TADF) have been spotlighted as a promising method to improve OLED performance.[3] HF mechanisms are enabled by interaction between TADF and TE which ultimately maximize emission efficiency and color purity. Moreover, multiple resonance (MR) emitter as TE may cause low spin-flipping activity to further push quality of emission. However, typical MR materials exhibit rigid planar molecular structure which limits color purity and quantum efficiency. Therefore, this study investigated the effects of functional groups (X) within CzBN which is a representative MR emitter.[4] Photoluminescence (PL) analysis confirmed suppression of excimer formation in high doping concentrations with films based on CzBN1 and 2 doped with HDT-1 in mCBP. In addition, molecules characterization was adopted to verify the effect of substituents on photophysical and device properties. Based on these results, mitigating planarity of the molecular structure for MR emitter is a promising strategy for improving HF based OLEDsReferences[1] C. Adachi et al., J. Appl. Phys., 90, 5048–5051 (2001).[2] H. Uoyama et al., Nature, 492, 234–238 (2012).[3] H. Nakanotani et al., Nat. Commun., 5, 4016 (2014).[4] Y.-T. Lee et al., Adv. Electron. Mater., 7, 2001090 (2021).


mCBP
HDT-1
CzBN1
CzBN2
CN
N
B
Photon Counts (I/I_0)
Time (h)
CzBN1 1 wt%
CzBN1 3 wt%
CzBN1 5 wt%
CzBN2 1 wt%
CzBN2 3 wt%
CzBN2 5 wt%
1.00
0.95
0.90
0.85
0.80
0
20
40
60
80

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-398**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Co nanoparticles using inverse micelle methods

Yu Bin Heo, Myung Jong Kim[1,*]

Gachon University Global Campus, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

Carbon nanotubes (CNTs) have been extensively studied in recent years in various fields. Since a transition metal catalyst is involved in the synthesis of carbon nanotubes, and the nano-diameter catalyst is related to small-diameter carbon nanotubes, it is important to synthesize small-diameter nanoparticles with a narrow size distribution. In this experiment, nanoparticles were synthesized using the inverse micelle method among various nanoparticle synthesis methods. The reverse micelle method is a method in which nanoparticles are synthesized by the reverse micelle formed by the surfactant in the water-in-oil microemulsion. It is effective in controlling the size of nanoparticles as the size of reverse micelles formed within various microemulsion compositions changes, and the nanoparticles are stabilized by DDAB on the surface of the nanoparticles. Through TEM and HRTEM analysis, it was confirmed that particles with an average diameter of 3-4 nm and a lattice of Co were synthesized. CNT was grown using the synthesized stable Co nanoparticles as a catalyst, and this was observed through TEM analysis. Through this study, it was shown that the size of Co nanoparticles can be efficiently controlled through the inverse micelle synthesis method, and these particles can serve as a catalyst in CNT growth.

Poster Presentation : **MAT.P-399**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Antimonene-Graphene Composite: A Versatile Electrocatalyst for Nitrogen Reduction and Beyond

Bo Gyeom Cho, In Young Kim[1,*]

Chemistry and Nano science, Ewha Womans University, Korea

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

Antimonene, a monoelemental 2D material belonging to Group VA, has garnered significant attention for its predicted exceptional stability and extraordinary electronic properties. However, the synthesis of hexagonal antimonene with high-quality and large-surface area has been impeded due to various challenges, hampering progress in this field.Previous studies have explored the synthesis of hexagonal antimonene utilizing halogen elements for desired anisotropic growth in a solution phase. However, a major hurdle has been the elimination of chlorine or bromine residues present on the antimonene surface.To address this limitation, we propose a novel approach involving utilization of graphene as a growth substrate for antimonene. Herein, we successfully prepared few-layer hexagonal antimonene and graphene composite by employing antimony(III) acetate and silane-modified graphene powder. Toluene was selected as the solvent for the graphene solution, which was carefully separated in a burette positioned above the flask to minimize thermal contact. Oleylamine was chosen as the reducing agent, and dodecylthiol served as a ligand to restrict lateral growth. This methodology also enables the creation of an antimonene-graphene nanocomposite.The experimental outcomes presented herein offer a promising and straightforward route for synthesizing antimonene-graphene composite, demonstrating their potential for widespread utilization due to the extraordinary electronic properties of hexagonal antimonene and graphene. Moreover we anticipate a great synergy of highly proficient in electrochemical abilities in these two 2D materialFurthermore, the formation of the antimonene-graphene nanocomposite holds the potential for enhanced electrocatalytic functionality for Nitrogen Reduction Reaction and exceptional properties, further expanding applications of this intriguing material.

Poster Presentation : **MAT.P-400**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Controlled catalysts for single-walled carbon nanotubes growth

Minseo Kim, Myung Jong Kim[*]

Department of Chemistry, Gachon University Global Campus, Korea

Single-Walled Carbon Nanotubes (SWCNTs) are a prominent material in modern nanotechnology due to their exceptional tensile strength, remarkable elasticity, superior thermal conductivity, high current-carrying capacity, and electronic properties spanning from metal to semiconductor. However, since the number of walls and diameter of nanotubes are directly affected by catalysts during the growth of CNTs, it is very important to maintain the small size and uniformity of catalysts by effectively controlling the heat-aggregation of catalysts during the Chemical Vapor Deposition (CVD) process. In this study, a method for physically controlling the heat-aggregation of deposited iron catalysts was devised by coating them with different materials (metals or h-BN). By using coated-iron catalysts, CNTs were grown through the CVD process and analyzed with Raman spectroscopy to examine the Radial Breathing Mode (RBM) peak and the D/G ratio of grown CNTs. Moreover, additional analyses with Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM) were conducted to measure the thickness and morphology of grown CNTs. This study aims to enhance the understanding of the synthesis of SWCNTs and to contribute to the exploration of potential future applications.

Poster Presentation : **MAT.P-401**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Catalyst Plasma Treatment for the CVD synthesis of BNNTs

DongHwan Lee, Myung Jong Kim*

Department of Chemistry, Gachon University Global Campus, Korea

Boron nitride nanotubes (BNNTs) are new materials attracting attention due to their exceptional properties, including outstanding mechanical strength, superior thermal stability, high thermal conductivity, and insulating and radiation shielding properties. However, BNNTs are mainly synthesized with high-temperature and high-energy methods such as plasma and laser ablation. The possibility of the mass production of BNNTs at low temperatures is being explored using the chemical vapor deposition (CVD) method with supported catalysts. In this study, "a catalyst-only reduction pathway" is provided for completely oxidized supports and catalysts by plasma treatment using PE-CVD (plasma-enhanced CVD) method. The length and yield of BNNTs synthesized with the hydrogen plasma-reduced catalysts are higher than those of BNNTs synthesized by the conventional CVD method. The synthesized BNNTs were analyzed using a Transmission Electron Microscope (TEM) and Scanning Electron Microscope (SEM). The ultimate goal of this study is to facilitate the large-scale synthesis of BNNTs with a high aspect ratio by using the CVD method.

Poster Presentation : **MAT.P-402**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Preparation of Ni-Pd/MgO-based bimetallic supported catalysts by wet-impregnation methods

Mingyu Shin, Myung Jong Kim[1,*]

Chemistry, Gachon University Global Campus, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

Carbon Nanotubes (CNTs) and Boron Nitride Nanotubes (BNNTs) have been of interest to many researchers in the field of nanotechnology due to their exceptional properties like high conductivity, superior mechanical strength, and remarkable thermal stability. To further expand the practical use of nanotubes in a variety of application fields, methods for the large-scale synthesis of high-quality nanotubes must be developed. Catalytic Chemical Vapor Deposition (CCVD) on supported catalysts is one of the methods with the potential to synthesize high-quality nanotubes in large quantities. To induce the growth of high-quality nanotubes, bimetallic transition metal catalyst particles must possess small diameters and must be in the form of uniformly dispersed alloy on the surface of the support material. In this study, Ni-Pd/MgO catalyst was synthesized with a newly devised wet impregnation method and analyzed with Transmission Electron Microscope (TEM). The results showed that nickel and palladium particles in newly synthesized Ni-Pd/MgO catalyst appeared to have reduced diameter, and enhanced uniformity and dispersity compared to Ni-Pd/MgO catalyst synthesized by the conventional wet-impregnation method. Furthermore, Energy Dispersive X-ray Spectroscopy (EDS) mapping data showed that the alloy of bimetallic catalyst particles was formed in a newly synthesized Ni-Pd/MgO catalyst. This study aims to improve the understanding of pathways for the synthesis of supported catalysts with the alloy of small, uniform, and highly dispersed bimetallic catalyst particles.

Poster Presentation : **MAT.P-403**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of W-BN core-shell nanoparticles using Arc discharge method for radiation shielding applications

Juseong Park, Myung Jong Kim[1,*]

Department of Nano Science and Technology Convergence, Gachon University Global Campus, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

The composition of boron or boron compounds with high-density elements has been confirmed by several studies as an effective double shielding of neutrons and gamma rays. In this study, the synthesis and coating of nanoparticles were prepared by an in-situ process to prepare core-shell nanoparticles in the form of boron nitride wrapped around the surface of core tungsten and dispersed in BP epoxy to fabricate hybrid composite shielding materials. The synthesized nanoparticles were analyzed by TEM, EDS, XRD, and XPS, and confirmed to be core-shell with a tungsten-boron nitride composition by FFT and HRTEM, based on the presence of W-B bonds and a small proportion of tungsten boride. This tungsten-boron nitride core-shell structure has the dual effect of improving the thermal stability of tungsten particles and attenuating the trapped gamma rays generated by the thermal neutron capture of boron nitride. This high double shielding performance is due to the fact that the tungsten core particles can effectively shield the capture gamma rays emitted during the thermal neutron capture process of 10-boron.

Poster Presentation : **MAT.P-404**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Novel Metal-BNNT Hybrid Materials: Synthesis, Characterization, and Prospects for Gamma Ray Shielding Applications

Honggu Kim, **Myung Jong Kim**[1,*]

Gachon University, Korea

[1]*Department of Chemistry, Gachon University Global Campus, Korea*

Boron nitride nanotubes (BNNTs) have captured substantial attention recently due to their exceptional characteristics such as elevated thermal conductivity, mechanical robustness, and remarkable chemical resilience. In this study, the infusion of WO_3 into BNNTs was employed to produce a composite amalgamation of metal and BNNTs, synergizing the advantageous attributes of both components. By confining WO_3 within BNNTs, a novel hybrid structure was fabricated and subjected to diverse analytical methodologies including SEM, TEM, and XRD for comprehensive evaluation. EDS mapping through TEM analysis unveiled the proficient dispersion of WO_3 within BNNTs, thereby validating the successful integration of WO_3 into the BNNT framework. Exploitation of the synthesized hybrid construct for potential gamma ray shielding applications was also undertaken. The outcomes underscore the auspicious shielding properties of the material, thereby motivating forthcoming endeavors aimed at refining its traits to optimize its suitability for this specific application.

Poster Presentation : **MAT.P-405**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ultrathin rGO/RuO_2/TiO_2 Hollow Nanospheres with Boosted Pseudocapacitive Charge Storage as Anode for Lithium-Ion Batteries

Ji-Ho Park, Seung-Min Paek[*]

Department of Chemistry, Kyungpook National University, Korea

The molecular-scale manipulation and combination of materials with different physical and electrochemical properties is one of the most promising strategies for the development of advanced secondary battery anode materials. In this study, we synthesized reduced graphene oxide/ruthenium oxide/titanium oxide hollow spheres (rGO/RuO_2/TiO_2-HS) fabricated via layer-by-layer self-assembly of exfoliated nanosheets. The high electrical conductivity of RuO_2 compensates for the low conductivity of TiO_2, and the robust structure of TiO_2, which resists volume expansion during the Li-ion insertion/desertion process, was expected to complement the drawbacks caused by the conversion reaction of RuO_2. The large surface area of hollow spheres facilitates the ion diffusion and access of electrolytes. In addition, The GO matrix in the hierarchical nanostructures increased the structural stability of the hollow sphere and blocked the particle growth of metal oxides during the heat treatment process. Accordingly, the large surface areas of rGO/RuO_2/TiO_2-HS led to exceptional Li-ion storage through pseudocapacitive behaviors and exhibited high capacity beyond the theoretical capacity of the physical mixture.

Poster Presentation : **MAT.P-406**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Adsorption of linear alpha olefins (LAOs) from olefin/paraffin binary liquid using ZIF-8 and ZIF-67: Experiment and Simulation

Sungbin Jo, SungHyun Yun[1], Yongchul Chung[1], Chung-Yul Yoo[*]

Department of Chemistry, Mokpo National University, Korea

[1]*Chemical & Biomolecular Engineering, Pusan National University, Korea*

Linear alpha olefins (LAOs) are linear hydrocarbons with one double bond at the edge of the molecular structure. LAOs are widely used as raw materials in petrochemical industry, such as surfactants and plasticizers. However, the major obstacle to obtain high-purity olefins is the separation and purification of olefin from olefin/paraffin mixture. In this study, selective adsorption of olefins from two olefin/paraffin mixture, 1-octene/*n*-octane (C_8) and 1-decene/*n*-decane (C_{10}), by zeolitic imidazolate framework (ZIF) has been investigated using batch adsorption experiments and configurational-biased grand canonical Monte Carlo (CB-GCMC) simulations using RASPA 2.0 program. Adsorption capacity and selectivity were obtained from the batch adsorption experiments. Adsorption sites, energy, and density of ZIF were calculated from the CB-GCMC. In addition, the results of batch experiments and CB-GCMC calculations were compared and discussed.

Poster Presentation : **MAT.P-407**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Selective synthesis of BNNTs and MgO-BN Core/Shell Nanowires by controlling catalysts

Chunghun Kim, Myung Jong Kim[1,*]

Department of Nano Science and Technology Convergence, Gachon University Global Campus, Korea
[1]*Department of Chemistry, Gachon University Global Campus, Korea*

The synthesis of boron nitride nanotubes (BNNTs) has attracted attention due to their superior mechanical properties, heat resistance, thermal conductivity, insulation, and potential for radiation shielding. Currently, high temperature and high energy methods with low synthetic volumes dominate the synthesis of BNNTs, but chemical vapor deposition (CVD) with supported catalysts holds promise for low temperature mass production. In this work, we introduce a controlled approach to prepare pure BNNTs and MgO-BN core/shell nanowires by modulating the oxidation level of the MgO support in CVD. A Ni-Pd alloy catalyst was used to improve the yield of BNNTs and MgO-BN core/shell nanowires, and characterization by electron microscopy, XRD, and thermogravimetric analysis confirmed their crystallinity and thermal stability. In addition, a simple treatment of MgO-BN nanowires with acid yielded BN fibers, which are similar to BNNTs but more easily scalable for synthesis. The utilization of CVD with a supported catalyst is expected to be a promising means for large-scale low-temperature production of BNNTs and derivatives.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-408**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Effect of the triplet state energy of organic guest on sensitizing the luminescence of Eu3+ and Tb3+ in layered yttrium hydroxide host

Yoonjae Choi, Song-ho Byeon[1,*]

Applied Chemistry, Kyung Hee University, Korea

[1]Department of Applied Chemistry, Kyung Hee University, Korea

Recently, the layered rare earth hydroxides (LRHs) with the general formula [RE2(OH)5(H2O)n]·X (RE = rare earths and X = interlayer organic and inorganic anions), have attracted much attention as another family of anionic clay consisting of rare earth cations to apply for a host system available for a wide range of photo and bioactive guest anions. However, because of low extinction coefficients of forbidden 4f‒4f intraconfigurational radiative transitions, the efficiency of direct electronic transitions for REs is intrinsically low and the energy transfer from sensitizers is required for the strong luminescence. Fortunately, high accessibility of diverse guest molecules to the interlayer gallery of LRHs could lead to organic/LRH hybrid materials accomplishing dramatically enhanced photoluminescence. In this work, layered yttrium hydroxides doped with Eu3+ and Tb3+ (LYH:Eu3+ and LYH:Tb3+) were selected for the inorganic host matrix to evaluate the sensitization efficiency of organic guest molecules intercalated into the interlayer gallery. The sensitization of RE3+ luminescence in this matrix is generally induced by UV-light energy absorption (π → π* transition) of organic molecule and subsequent intersystem crossing to its lowest triplet (T1) state, followed by the energy transfer to the lowest excitation state of RE3+ ions. Considering the 5D0 excited state of Eu3+ (17,250 cm−1) and the 5D4 excited state energy of Tb3+ (20,545 cm−1), organic sensitizers having T1 state energies in the range of 19,000~23,000 cm-1 were selected as the interlayer guest to investigate the photoluminescence of Eu3+ and Tb3+ as a function of their T1 state energy.

Poster Presentation : **MAT.P-409**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Exfoliation of N-rich Carbon Nitrides with Tailored Band Structures

Ayoung Yoon, In Young Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Graphitic carbon nitride (g-C3N4) has been studied in various fields due to its high chemical stability, facile synthesis, and relatively low cost. It has also been studied in research for electrocatalytic applications, because it has semiconductor properties due to its bandgap (2.7 eV) and has a nitrogen-rich carbon framework. 2D g-C3N4 shows better activity than bulk g-C3N4 because its abundant structural defects and surface terminal groups play an important role in catalytic activation. In this work, we exfoliate not only g-C3N4 but also N-rich carbon nitrides such as C3N4.8, C3N6 and C3N7 through a sonochemical process. The resulting colloidal suspensions of N-rich carbon nitrides show a distinct Tyndall effect, indicating successful exfoliation of the carbon nitrides. Transmission electron microscopy (TEM) reveals that lateral size of the exfoliated nanosheets is hundreds of nanometers. Zeta potential analysis demonstrates that all the exfoliated N-rich carbon nitride nanosheets present negative surface charges. Near edge X-ray absorption fine structure (NEXAFS) spectroscopy for the N-rich carbon nitride nanosheets confirm that triazole-based structures of the carbon nitrides are well maintained after exfoliation. Interestingly, the maximum absorption wavelength of the exfoliated C3N4.8, C3N6 and C3N7 nanosheets are blue-shifted as compared to g- C3N4 nanosheets, which is examined by UV-Vis absorption spectroscopy and photoluminescence spectroscopy. We plan to utilize stably exfoliated carbon nitrides in a nitrogen reduction reaction.

Poster Presentation : **MAT.P-410**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Toward non-gas-permeable hBN film growth on smooth Fe surface

Hayoung Ko, Soo Min Kim[1,*]

Energy Science, Sungkyunkwan University, Korea

[1]*Chemistry, Sookmyung Women's University, Korea*

Hexagonal boron nitride (hBN) has been highlighted due to its high optical transparency in the visible range and high-temperature oxidation resistance up to 1500 ℃ in air [1]. Typically, large-area m-hBN films have been synthesized on Fe-based substrates due to reasonable B and N solubilities in Fe bulk [2-4]. In this precipitation stage, rough Fe surfaces composed of atomic grooves, steps, and kinks on a Fe grain in polycrystalline Fe foil produce a non-uniform and discontinuous polycrystalline hBN film [2, 3]. Thus, an atomically flat surface is desirable to achieve a high-quality m-hBN film.In this study, we report an effective growth method to improve the quality of m-hBN in terms of its uniformity and continuity by using a smooth Fe surface. The smooth Fe surface allows the uniform precipitation of B and N to grow highly uniform and continuous m-hBN films. Further, the m-hBN/Gr heterostructure film exhibits impressive WVTR performance with high transparency compared to previously reported values.

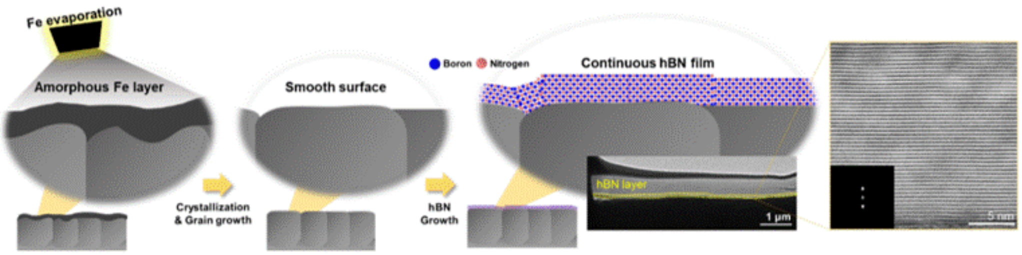


Fig.1 Schematic illustration of this concept and the cross-sectional TEM images.

Poster Presentation : **MAT.P-411**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Fabrication of Implantable Electrochemical Sensors using Conformal Biocompatible Material Coating

Jiae Park, Kwanwoo Shin[1,*]

Chemistry, Sogang University, Korea

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

In recent years, the demand for real-time and minimally invasive monitoring of physiological paramters within living organisms has driven significant advancements in biosensor technology. However, a significant portion of these biosensors utilize fabrication techniques borrowed from the semiconductor industry, leading to disparties in materials, mechanical properties, and profiles compared to the flexible nature of biological tissues. In this study, we introduce an improving approach by developing a diffusion-based electrochemical sensor, coated with alginate and gelatin, specifically designed for in vivo sensing applications. Alginate and gelatin has good biocompatibility, biodegradability, nontoxicity, and hydrophilicity. The conductive gel ink made of CaCl2, and carbon nanotubes(CNTs), which is extruded onto a mixture of alginate and gelatin. The calcium ions in the CNT-Ca2+ diffuse and crosslink with the alginate to produce a coated construct. The use of alginate and gelatin is particularly advantageous due to their similar mechanical properties to biological tissues, rendering them biocompatible coatings suitable for implantable electrochemcial sensors.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-412**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Formation of Electrospun Keratin Nanofibers: Protein Structure, Mechanical and Chemical Properties for Food packaging

Kim SuGyoem, Kwanwoo Shin[1,*]

Chemistry, Sogang University, Korea

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

Keratin is one of the most abundant materials readily available from natural resources, 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 chemical stability, particularly when compared to other materials. These distinctive properties of naturally derived keratin can be leveraged to create nanofibers through the process of electrospinning for direct application in food coatings. Fibrous materials prepared via electrospinning hold the advantage of possessing a high surface area to volume ratio. They can be coated on various types of surfaces, and can even incorporate additional active substances such as antimicrobial agents if needed. In this study, we have identified the conditions for forming fibers through electrospinning naturally derived keratin. We aim to determine the internal structure of the uniformly formed fibers, especially the protein structure, as well as their mechanical and chemical properties. This research aims to utilize the intrinsic advantages of keratin alongside the benefits of nanofibers, aiming for their application in future advancements in food packaging.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-413**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Development of Drug carrier Using Silk Fibroin Encapsulated Hydroxyapatite Hybrid material

Byeongho Park, Sehun Jung, Seog Woo Rhee*, Jinkwon Kim*

Department of Chemistry, Kongju National University, Korea

In this study, organic-inorganic hybrid particles were obtained by combining Hydroxyapatite (HAP), a primary component found in living organisms' bones, and Silk fibroin (SF), a natural polymer sourced from silkworm cocoons. The characterization of the crystalline structure of HAP and the presence of SF have been done using various instrumental analysis such as XRD and FT-IR. The size and morphology of as-synthesized particles were determined by SEM images. TGA was used to assess drug loading in the complex, while drug release was determined by UV-Vis analysis in a phosphate buffer solution (PBS).

Poster Presentation : **MAT.P-414**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

A study intercalated anion effect on flame retardancy of the composite materials of clay mineral natural and silk fibroin for the traditional Hanji

Sehun Jung, **Seog Woo Rhee***, **Jinkwon Kim***

Department of Chemistry, Kongju National University, Korea

In this study, an eco-friendly flame retardant was developed in an aqueous media using clay minerals and silk fibroin. A synthetic hydrotalcite containing various anions such as carbonate, phosphate, and molybdate were prepared for a new kind of clay mineral pigment. Silk fibroin was extracted from cocoons and used as a natural organic binder and coating agent. The thermal decomposition behaviors of the composites were monitored by thermal analysis (TGA/DSC). Combustion tests were performed from 200 ℃ upto 600 ℃ using a microcalorimeter with a paper specimen coated with a composite pigment by a dip coating method. The flame retardancy of the specimen was investigated by measuring the heat release rates (HRR) and the oxygen consumption amounts as a function of time.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-415**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Exploration of $Na_{2+x}Zr_{1-x}M_xCl_6$ Solid Electrolytes as Potential Catholytes for Sodium Solid-State Batteries

Dongyeon Yun, Seung-Tae Hong*

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea

All-solid-state batteries (ASSBs) have emerged as alternatives to conventional lithium-ion batteries, garnering significant attention in recent years. ASSB is composed of two electrolytes: a solid electrolyte responsible for efficient ion transport and membrane function, and a catholyte integrated into a cathode composite. Recently, various studies on halides as catholytes have been conducted due to their chemical stability with oxide-based anode materials. In this work, a series of $Na_{2+x}Zr_{1-x}M_xCl_6$ solid solutions are prepared through high energy ball-milling and subsequent annealing processes conducted at various temperatures. The substitution system, based on Na_2ZrCl_6, were formed in the compositional range of $x = 0.0$ to 0.5. The Rietveld refinement analysis showed the successful substitution and the increase in Na occupancy. Remarkably, the ionic conductivity increased almost 10 times at $x = 0.2$ compared to the pristine material. This improvement indicates the positive influence of the increasing Na occupancy on the ion transport properties. This study offers insights into the potential utilization of $Na_{2+x}Zr_{1-x}M_xCl_6$ solid electrolyte as a catholyte component in high-performance solid-state batteries.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-416**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Defect-controlled ultrathin large-area 2D holey metal nanosheets with efficient electrocatalyst performance

Xiaoyan Jin, Seong-Ju Hwang[*]

Department of Materials Science and Engineering, Yonsei University, Korea

Elemental metal nanostructures have evoked a great deal of research efforts because of their unique physicochemical properties and valuable functionalities. Here we report a novel synthetic route to ultrathin 2D holey Ru nanosheets with atomic-level thickness and surface holes via the finely-controlled thermal reduction of exfoliated RuO_2 monolayer at elevated temperature. The obtained Ru nanosheets show extremely high morphological anisotropy with ultrathin thickness of ~1.0 nm, huge lateral dimension with micrometer size, and controllable size of surface holes. This is the first example of ultrathin holey metal nanosheets with extremely high morphological anisotropy. The alteration of reduction condition enables to optimize the electrocatalyst performance of Ru metal nanosheets via the fine-tuning of defect structure. The obtained holey Ru nanosheets deliver higher electrocatalytic activity for hydrogen evolution reaction (HER) in 1.0 KOH electrolyte than those of Pt/C and bulk Ru metal. The beneficial effect of holey nanosheet formation on the HER electrocatalytic activity can be ascribed to the creation of crystal vacancies, the provision of many surface sites, and the improvement of mass transport.

Poster Presentation : **MAT.P-417**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Interaction-based Bacteria-dye Combination Screening for Visualization of *Acinetobacter baumanni*

Ji Hye Jin, Dokyoung Kim[1,*]

Department of Biomedical Science, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Bacterial identification is crucial for accurate clinical diagnosis and effective treatment, especially in the face of antibiotic-resistant strains. We introduce an innovative screening approach that uses tailored fluorescent dyes for precise and rapid detection of bacteria. BMeS-p-A is a positively charged dye that contains a diamine group and a benzothiazole moiety. It shows exceptional selectivity in fluorescence staining for Gram-negative *Acinetobacter baumannii* (AB) and its carbapenem-resistant form (CRAB), by interacting with their negatively-charged surface. We characterized the photophysical properties, sensing capabilities, and potential antibiotic properties of BMeS-p-A. Also, we demonstrated the application of BMeS-p-A for imaging the biofilm formation of AB and CRAB on urinary catheters, which are widely used medical devices that can facilitate bacterial colonization and infection. This pioneering application addresses the pressing concern of bacterial colonization and related infections associated with medical devices. We hope this study inspires future research and innovative approaches to combat bacterial threats and the mounting challenge of antibiotic resistance.

Poster Presentation : **MAT.P-418**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Silver Telluride Colloidal Quantum Dot Photodetector in Near-Infrared Region

Gahyeon Kim, Dongsun Choi, So Young Eom, Jin Hyeok Lee, Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

Silver chalcogenides colloidal quantum dots (CQDs) are well-known non-toxic candidates that exhibit the excitonic feature from the near-infrared (NIR) to extended short-wavelength infrared (eSWIR) region. The thiol-ligands, which mainly stabilize the surface of the Ag2Te CQDs, have limited further ligand exchange procedures, leading to the various applications using the CQD films. Here, we report non-toxic and ambipolar silver telluride (Ag2Te) CQD inks by engineering the thiol-free surface of QDs with a suitable combination of silver metal and ligands, allowing convenient fabrication. The Ag2Te CQD inks-based infrared homojunction photodetector with an external quantum efficiency (EQE) was measured at 1.7 μm. The Ag2Te CQDs photodetector devices exhibiting the greatest EQE at 1.7 μm will provide further opportunities for infrared optoelectronic, biosensing, and telecommunication applications with low toxicity.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-419**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Mercury Telluride Colloidal Quantum Dot Based High-Sensitive Mid-wavelength Infrared (MWIR) Photodiode Sensors

So Young Eom, Haemin Song, Gahyeon Kim, Yoon Seo Jung, Dongsun Choi, Jin Hyeok Lee, Hyeong Seok Kang[1], Jiyeon Ban, Woong Kim[2], Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

[1]chemistry, Korea University, Korea

[2]Division of Advanced Materials Engineering, Korea University, Korea

Colloidal quantum dot (CQD) photodetector has been rigorously investigated due to the low-cost manufacturing process, fast response time, and high sensitivity of devices. Furthermore, tunable bandgap and intra-bandgap energies of the CQDs, which is a unique property of the CQDs, enable us to exploit a wide range of light from UV to mid-wavelength infrared (MWIR) for light-to-electricity conversion. We successfully fabricated the MWIR CQD photodiode by incorporating synthesized p-doped HgTe nanocrystals (NCs). As a result, the thermal images were successfully obtained using MWIR photodiode sensors.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-420**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Colloidal Tellurium Nanowire Laser in the Mid-Wavelength Infrared Region

Jin Hyeok Lee, Gahyeon Kim[1], Dongsun Choi[2], Kwang Seob Jeong[2,*]

Chemistry, Korea University, Korea

[1]*Korea University, Korea*

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

Colloidal infrared emitters in the mid-wavelength infrared (MWIR) can be widely used for various applications such as low-power IR light-emitting diodes (LEDs), sensors, deep-tissue imaging, and infrared spectroscopy. Here, we present the colloidal tellurium nanowires (Te NWs) that show a strong emission intensity in the mid-wavelength infrared region at room temperature. As the temperature decreases to 78 K, the full-width-half-maximum (FWHM) narrows, and the emission intensity dramatically increases, which comes from the lasing property. We realized the band gap tunable of Tellurium nanocrystals with the varying synthesis conditions. Suggesting that the band gap of Te nanocrystals can develop a large energy region.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-421**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

A phase tuning approach to optimize electrocatalyst performance of MoS_2 nanosheets

Dong Wook Lee, Xiaoyan Jin, So Yeon Yun, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

Transition metal dichalcogenides have attracted tremendous research interest owing to their useful functionalities as noble-metal-free electrocatalysts. Despite of numerous advantages of transition metal dichalcogenides, these materials suffer from critical limitations such as structural instability and insufficient activity. In effort to enhance the applicability of transition metal dichalcogenides, we develop a phase-tuning approach of interlayer-expanded MoS_2 nanosheets via defect-assisted boride substitution. The $NaBH_4$ treatment for tetrapropylammonium-restacked MoS_2 nanosheets allows to substitute boride ions into the anion vacancies of MoS_2 nanosheets due to formation of coordinate bonds with the Mo defect sites. The boride substitution results in an increase in concentration of active sites for hydrogen evolution reactions. Additionally, the resultant adjustment of 1T'/2H phase ratio improves structural stability and charge transfer kinetics. The present defect-assisted boride substitution approach can provide an effective method to explore high-performance noble-metal-free electrocatalysts.

Poster Presentation : **MAT.P-422**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Engineering Porous Structures of Cu/C Nanofibers for CO_2 Reduction Electrocatalysts

Daewon Bae, Dae-Hyun Nam[1,*]

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

[1]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Electrochemical CO_2 reduction reaction (CO_2RR) is a promising solution for carbon utilization that can convert CO_2 into value-added fuels and chemicals. Copper (Cu) is the element which can induce *CO dimerization to produce C_2 products such as ethylene and ethanol. Catalyst supporters are essential to stabilize the active materials and reduce agglomeration of them. Carbon (C) supporters exhibit high porosity, high electric conductivity, and stable under reductive potential. However, it is still unclear to understand the role of the porous structures of C supporters on CO_2RR. In this work, we report a methodology to utilize C supporter as not only porous structures but also a template to optimize the structures of Cu active materials toward efficient ethylene production by CO_2RR. This was due to the formation of hierarchical porous C structures by heterogeneous interfaces between dual polymers and separated redox of Cu and C with selective carbon combustion. To control the C porosity, we utilized the polymers having different thermal decomposition behaviors. In addition, we controlled oxygen partial pressure (pO_2) during calcination for selective combustion without Cu oxidation. We figured out that the higher porosity of C supports formed by synergistic effects of sacrificial polymer-induced pores and selective combustion promotes ethylene productivities compared to C supports with lower porosity; about 2-fold enhancement of ethylene Faradaic efficiency in 1 M KOH electrolyte. Further studies will be discussed to unveil how the porous C supporters affect the microenvironments to trigger ethylene formation.

Poster Presentation : **MAT.P-423**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Ionic conductivity measurement of wurtzite $Li_{2.95}Al_{0.95}Si_{1.05}O_5$ depending on the compaction processing

Song Hyeon Kim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

Complex wurtzites $Li_{3-x}Al_{1-x}Si_{1+x}O_5$ exhibit moderate ionic conductivities of $10^{-5.5}$ ~ $10^{4.6}\Omega^{-1}$ cm^{-1}, depending on x, at 500 °C. In this study, the effects of sample processing on the conductivity evaluation were examined using $Li_{2.95}Al_{0.95}Si_{1.05}O_5$. Particularly, the sintering temperature, flux additive B_2O_3, and the type of electrode contact (Ag, Au, In-Ga) were used as the control parameters. The polycrystalline morphology and the ac impedance spectral characteristics are to be compared.

Poster Presentation : **MAT.P-424**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Boosting Hydrogen Evolution Reaction through Strained rGO/MoS2/PS Electrodes

Kang Ji-Hun

Chemistry, Kyung Hee University, Korea

The hydrogen evolution reaction (HER) is a reduction process of water which can produce hydrogen energy, gaining significant attention as an environmentally friendly technology to replace fossil fuels. Previous studies employed noble metal catalysts like Pt, Ir, and Ru for the HER. However, the high cost of these noble metal-based catalysts hampers their commercial viability. To enhance the HER performance, increasing active sites and facilitating effective charge transfer are essential to improve kinetics and achieve low overpotential. Recently, two-dimensional (2D) materials such as graphene and MoS2 have emerged as promising alternatives to noble metals for HER catalysts. These materials offer comparable performance at a low cost. In this study, we synthesized a MoS2/rGO film to provide a large surface area and active sites. The electrochemical HER performance of the rGO/MoS2/polystyrene (PS) electrode was evaluated by heat-induced shrinking of polystyrene substate. Strained rGO/MoS2/PS electrodes exhibited improved HER performance compared to the unstrained counterparts, displaying an overpotential of 175 mV at a current density of j = -3 mA cm-2 and maintainging stability for over 10 hours. In conclusion, our findings suggest that the strained rGO/MoS2/PS electrode enhances HER performance, offering a novel approach to HER catalysts.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-425**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Electrochemical Behavior of Graphene Grown on Cu Depending on the Different Types of Molecules

Minhyeok Kim, Sun Hwa Lee[1,*], Rodney Ruoff[2,*]

Center for Multidimensional Carbon Materials, Institute for Basic Science/UNIST, Korea

[1]*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

[2]*Center for Multidimensional Carbon Materials , Institute for Basic Science, Korea*

We present the electrochemical reactivity of graphene, which is dependent on the type of molecules. We used a simple electrochemical method to functionalize single crystal graphene on Cu(111) with various types of organic molecules containing iodide group, and probed the degree of functionalization by Raman spectroscopy. Our study revealed that the reactivity of graphene changes with the reagents, and that molecules with functional groups having reactive sites had no reaction with graphene or even caused side reactions on the graphene. In contrast, molecules with no reactive groups showed an increased degree of reaction with the applied potential. Our findings provide a deeper understanding of the electrochemical behavior of graphene and demonstrate a general method to functionalize graphene with a broad range of organic molecules. This work is supported by the Institute for Basic Science (IBS-R019-D1).

Poster Presentation : **MAT.P-426**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Molecular Structural Descriptor-assisted Machine Learning to Accelerate Development of Organic Photovoltaics

Gyu-Hee Kim, Doo-Hyun Ko[1,*]

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

Although organic photovoltaics (OPVs) have made significant progress over the last two decades, the discovery of new materials and device optimization for high-performance remains challenging, due to their numerous considerations. In order to reduce this labor-intensive trial-and-error approach and expedite the advancement of OPVs, machine learning (ML) coupled with quantitative structure-property relationships has attracted. The previous OPV-ML models are limited in their applicability as they require the accurate determination of material properties through measurement or calculation before using the models. Here, to streamline the laborious process, a unique descriptor platform that translate molecular structures into a concise matrix of integers is designed. Our concise and intuitive descriptor allows the ML models to comprehend molecular structures and prioritize each fragment that significantly contribute to the photovoltaic performance. Moreover, with the succinct descriptor system, we build the OPV ML models which can predict performance of both binary and ternary OPVs simultaneously. The proposed ML model achieves a high correlation coefficient of 0.86 between experimental and predictive power conversion efficiency of OPVs, despite using only the molecular structure information and composition ratio without any additional material property. Moreover, we assure the reliability of the descriptor platform and ML models through in-depth analysis and verification protocol. Therefore, this study proposes a highly accurate and reliable predictive OPV-ML platform that can robustly screen numerous candidates out and provide valuable guideline for the design of new promising materials.

Poster Presentation : **MAT.P-427**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

The growth of highly ordered, porous, and graphene-like 3D carbon under highpressure using FAU zeolite as a template and acetylene as a carbon source

Bayrammuhammet Annageldyyev, Madi Arsakay[1], Alisher Fatkhulloev[2], Won Kyung Seong[2], Sun Hwa Lee[2], Rodney Ruoff[3,*]

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Korea

[1]Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science, Korea

[2]Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea

[3]Center for Multidimensional Carbon Materials / Dep, IBS CMCM / UNIST, Korea

Chemical vapor deposition of carbon precursors inside zeolite particles under close-to-normalpresssures have has been a conventional way to synthesize Zeolite Templated Carbons (ZTCs). In this work,we have studied the synthesis of high-quality ZTCs under high-pressure (20 bar) conditions. C_2H_2 was used as a carbon precursor and Ca^{2+} exchanged FAU zeolite as a sacrificial template, obtaining a carbon-zeolite composite with high structural density, followed by the dissolution of templatematerial. Subsequently, a crystalline ZTC has been synthesized and characterized. This novel methodallowed us to eliminate the need to raise the growth temperature for the synthesis. To optimize thequality of the ZTC, we have also explored the effects of synthetic variables including zeolite counterion type, growth temperature and duration, and inlet flow rate. We (BA, MA, AF, WK, SH, RSR) appreciate thesupport from the Institute of Basic Science (IBS).

Poster Presentation : **MAT.P-428**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Photodetection Range Expansion through the Cation Exchange Method

Yoon Seo Jung, Kwang Seob Jeong*, Dongsun Choi, Haemin Song

Department of Chemistry, Korea University, Korea

Instead of the heavy metal-based mid-infrared active materials, silver selenide colloidal quantum dots (CQDs) have emerged as the alternatives showing the steady state intraband transition between $1S_e$ and $1P_e$ states. However, given that the intraband transition is confined solely to the mid-IR wavelength, it is a huge challenge to broaden the intraband transition to the higher energy states. In this work, we present the cation exchanged Ag_xSe (X>2) CQDs derived from the PbSe CQDs, which shows the intraband transition up to 0.39 eV. Application to the electrochemical luminescence and the intraband photodetectors has verified the steady state intraband transition in the cation-exchanged CQDs. The I-V characteristics and the on-off infrared photocurrent were measured from different device structures at various temperatures. This research underscores how the cation exchange method can effectively broaden the range of the intraband transition and the broad spectral range of the Ag_xSe CQDs will enhance its suitability for infrared detection applications.

Poster Presentation : **MAT.P-429**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Synthesis of Thermally Stable and Highly Luminescent Cs5Cu3Cl6I2 Nanocrystals with Nonlinear Optical Response

Dongil Son, Jongnam Park[1,*]

Graduate school of semiconductor materials and device engineering, Ulsan National Institute of Science and Technology, Korea

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

Research in the past decade has seen significant progress in lead (Pb) metal halide semiconductors for optoelectronics. However, their high toxicity and chemical instability hinder practical use. Alternative metal halide perovskites like Sn, Ge, Bi, and Sb have been proposed, but their luminous efficiencies fall short of Pb-based counterparts. The demand for next-generation metal halide semiconductors with superior quantum efficiency and stability is growing.This work introduces Cu(I)-based metal halide compounds as a viable substitute for Pb and Sn perovskites. These materials, noted for low toxicity and excellent stability, offer distinctive luminescence governed by self-trapped excitons (STEs). Notably, Cs5Cu3Cl6I2, an exemplar, demonstrates blue light emission, showcasing its potential as a frontrunner for future blue light-emitting applications.We have successfully developed a colloidal process to synthesize Cs5Cu3Cl6I2 NCs with a high luminescence efficiency (QY ≈ 100%) and thermal stability. Furthermore, we analyzed the impact of reaction parameter variations on the anisotropic growth of these NCs. Through halide engineering, we demonstrated the feasibility of modulating the energy levels of self-trapped excitons (STEs) in Cs5Cu3Cl8-xIx, thereby expanding its potential applications.In addition, we present the results of patterning research utilizing the exceptional optical characteristics of Cs5Cu3Cl6I2. High-resolution patterning is crucially investigated for potential applications in next-generation displays. We introduce pioneering patterned studies in the context of Pb-free perovskites and showcase security patterning outcomes leveraging the distinctive luminescent properties inherent to Cs5Cu3Cl6I2.

Poster Presentation : **MAT.P-430**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Enhancing Compatibility and Electrochemical Performance of All-Solid-State Batteries through Novel LISICON-Type Oxide Electrolytes

Suhyun Kim, Seung-Tae Hong[1,*]

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

[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

The focus on all-solid-state batteries (ASSBs) has been increasing due to their potential to replace flammable organic liquid electrolytes with safer non-flammable inorganic solid electrolytes (SEs). An essential condition for achieving elevated energy density in ASSBs is the simultaneous compatibility of SEs with electrode materials possessing high energy density, such as Ni-rich layered cathode materials and Li-metal anodes. Among the various options for SEs, oxide-based ones are noteworthy due to their chemical stability in ambient air and their lack of toxic gas release. Nevertheless, the adoption of oxide-based SEs presents challenges stemming from their rigid ceramic properties, leading to a high interfacial resistance between the cathode and electrolytes during the manufacturing process. This challenge is especially pronounced at room temperature, owing to poor contact at the interface. Additionally, the elevated sintering temperature required for oxide SEs triggers chemical reactions between the cathode materials and the oxide SEs. This results in the deterioration and loss of electrochemical activity in the cathode materials. In this study, we explore LISICON type oxide solid electrolytes that can be co-sintered with Ni-rich NCM cathode materials before reaching the point of NCM's degradation. The augmentation of electrochemical properties in LISICON-type SEs is achieved through the substitution of aliovalent metals. Through X-ray diffraction, we demonstrate the presence of impurities and the extent of disordering. Furthermore, we assess the electrochemical performance by using electrochemical impedance spectroscopy (EIS) and half-cell test. Additionally, we endeavor to construct an all-solid-state cell using dry coating techniques.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-431**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

A Study of Zn2GeO4@C with a core shell structure applicable to lithium-ion batteries

Deukhyeon Nam, Joon Ha Moon[1], Jaewon Choi[1], Chan Woong Na[2], Yoon Myung[2,*]

Korea Institute of Industrial Technology, Korea University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*Korea Institute of Industrial Technology, Korea*

Ge based materials have a theoretical high specific capacity, which is advantageous as an anode materials for lithium-ion batteries. However Ge has poor stability due to large volume changes during lithiation/delithiation process. In this work, we fabricated Zn2GeO4@C sphere with a core shell structure. Zn2GeO4 nanoparticles were synthesized by hydrothermal method and coated with resorcinol-formaldehyde resin by sol-gel method. After that, Zn2GeO4@C spheres were obtained by carbonization through annealing under Ar atmosphere. The structural properties of the Zn2GeO4@C were analyzed by using SEM, XRD, and raman. The Zn2GeO4@C spheres are expected to be used as lithium-ion batteries.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **MAT.P-432**

Material Chemistry

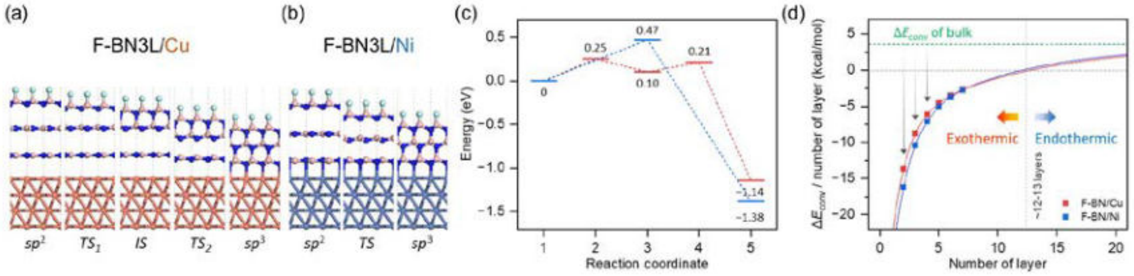
Exhibition Hall C FRI 11:00~13:00

Synthetic Way for Atomically Thin Wurtzite Boron Nitride via Periodic Functionalization

Joohee Oh, Hyunseob Lim*

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

In recent years, the exploration of two-dimensional materials has gained significant attention due to their unique properties and applications in various fields. Wurtzite boron nitride(w-BN) possesses several interesting properties rivaling those of diamond. Especially, owing to the high chemical stability, w-BN is desired for fabricating electronic devices that can withstand harsh environments. However, the realization of w-BN-based functional devices is still a challenging task due to the difficulty in the preparation of high-quality w-BN films with uniform thickness and controllable properties. Herein, we propose a synthetic way of w-BN by periodic functionalization which converts the sp^2 bonds of hexagonal boron nitride (h-BN) into sp^3 hybridization with the formation of interlayer bonds, using density functional theory (DFT) calculations. We investigated the conversion of bonds with representative substrates (copper and nickel) which are used in two-dimensional material synthesis and analyzed the various properties such as mechanical, optical, and electrical properties. Additionally, variations in trends have been identified between Cu and Ni substrates, and it has been confirmed that an exothermic conversion can be achieved by selecting the appropriate substrate. Our investigations suggest that the functionalization of two-dimensional materials provides a means of controlling properties.


(a)
F-BN3L/Cu
sp2
TS1
IS
TS2
sp3
(b)
F-BN3L/Ni
sp2
TS
sp3
(c)
Energy (eV)
0.5
0.0
-0.5
-1.0
-1.5
0
0.25
0.47
0.10
0.21
-1.14
-1.38
1
2
3
4
5
Reaction coordinate
(d)
ΔEconv / number of layer (kcal/mol)
ΔEconv of bulk
5
0
-5
-10
-15
-20
Exothermic
Endothermic
~12-13 layers
F-BN/Cu
F-BN/Ni
0
5
10
15
20
Number of layer

Poster Presentation : **MAT.P-433**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Facile and Low-energy Integration of Metal Electrodes with Two-dimensional Semiconductors Using the Electroless Deposition Process

Giyoon Kwak, Hyunseob Lim*

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

Two-dimensional semiconductors such as transition metal dichalcogenides (TMDs) have been studied as promising materials for future electronic applications. However, thermal/e-beam evaporation, a representative conventional metallization approach, has several problems in applying 2D semiconductors to advanced and novel applications. First, evaporation methods usually involve “high energy” metal atom or cluster bombardment. It can damage the atomically thin 2D semiconductors and restrict the use of materials that are vulnerable to heat or vacuum. Second, it is hard to deposit metals uniformly on complex-shaped surfaces. Third, expensive dedicated equipment is required.Here, we present facile and low-energy integration of metal electrodes with 2D semiconductors can be achieved by the electroless deposition process. By reducing metal ions on the surface of 2D semiconductors at relatively low temperatures, we achieve the “low energy” deposition of metals. Using these methods, we could measure the electrical properties of semiconductors from the patterned 2D TMDs field effect transistors. Furthermore, we could see the possibility that TMDs received less damage during the electroless deposition process than evaporation methods when we peeled off the deposited metals. Since electroless deposition does not require dedicated equipment, it has the advantage of being able to make 2D semiconductor devices easily. Furthermore, we expect the isotropic deposition nature of the electroless deposition enables us to deposit metal electrodes uniformly on the complex-shaped 2D semiconductor surfaces.

Poster Presentation : **MAT.P-434**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Facile Mesoporous Hollow Silica for Formaldehyde Adsorption

Jong-tak Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Formaldehyde emitted from household products is classified as a hazardous substance, that adversely affects human health, so recently, various studies related to adsorption materials for reducing formaldehyde have been widely reported. In this study, mesoporous and mesoporous hollow silicas introduced amine functional groups were utilized as an adsorption material for formaldehyde. Mesoporous and mesoporous hollow silicas with well-developed pores were compared in their formaldehyde characteristics based on their synthesis methods, which were with or without a calcination process. The best formaldehyde adsorption result was in mesoporous hollow silica synthesized through the non-calcination process and followed by the mesoporous hollow silica synthesized through the calcination process and the mesoporous silica in order of adsorption characteristics. This is because the hollow structure demonstrates better adsorption properties than mesoporous silica due to the large internal pores. Also, the specific surface area of the mesoporous hollow silica synthesized through the non-calcining process increased than one of the calcined processes, and it led to better adsorption performance. This research suggests a facile synthetic method of mesoporous hollow silica and confirms noticeable potential as a support for the adsorption of harmful gases.

Poster Presentation : **MAT.P-435**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

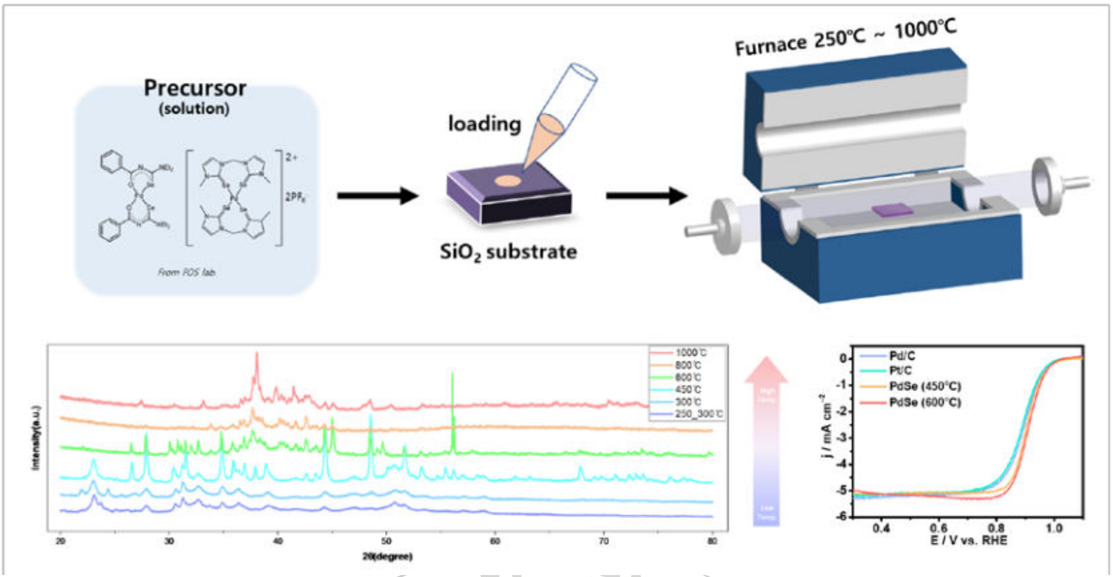
Synthesis and Application of Multiphase $PdSe_2$ Using Single Source Precursor

Hyeon Ju Kim, Hyunseob Lim[1,*]

chemistry, Gwangju Institute of Science and Technology, Korea

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

Two-dimensional palladium diselenide ($PdSe_2$) has received extensive attention as one of the promising materials for making devices because of its high carrier mobility (~158 $cm^2V^{-1}s^{-1}$), wide indirect bandgap variation (0eV at bulk ~ 1.3eV at monolayer), long-wavelength infrared photoresponsivity (～42.1 AW^{-1} at 10.6 μm), near-infrared photoresponsivity (660 AW^{-1} under 914 nm laser). In addition, as a catalyst containing palladium, Pd-Se with various phases (e.g., PdSe, $PdSe_2$, $Pd_{17}Se_{15}$, etc.) becomes an emerging research topic in oxygen reduction reaction (ORR).Here we synthesized multi-phase $PdSe_2$ by single-source precursor using chemical vapor deposition (CVD) method. By using a single organometallic precursor, a stoichiometric synthesis, uniform loading of samples through solvent application and simplification of reaction steps were expected. Additionally, It is possible to prevent waste of source powder, contamination of reaction tubes and generation of acid vapor due to the use of halide salts precursor which occur in a general chemical vapor deposition method of synthesizing $PdSe_2$ using separate Pd and Se sources. In this study, as it was confirmed that the composition ratio of Pd-Se changes depending on the synthesis temperature, the electrical properties and catalytic activity according to each temperature were observed. This provides an understanding of the synthesis of $PdSe_2$ using single-source precursors and a new electrocatalytic perspective on multi-phase $PdSe_2$.


Precursor
(solution)
From FOS lab
loading
SiO₂ substrate
Furnace 250℃ ~ 1000℃
1000℃
800℃
600℃
450℃
300℃
250_300℃
Intensity(a.u.)
20
30
40
50
60
70
80
2θ(degree)
Pd/C
Pt/C
PdSe (450°C)
PdSe (600°C)
j / mA cm⁻²
0
-1
-2
-3
-4
-5
-6
0.4
0.6
0.8
1.0
E / V vs. RHE

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-436**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Highly Enhanced Biocompatibility of Dexamethasone in Layered Double Hydroxide

Sieun Park, Goeun Choi[*], Jin-Ho Choy[1,*]

a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN)b.Department of Nanobiomedical Science and BK21 PLUS NBM Global Research Center for Regenerative Medicine, Dankook University, Korea
[1]*a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN)b.Division of Natural Sciences, the National Academy of Sciences, Seoulc.Department of Pre-medical Course, College of Medicine, Dankook University , Korea*

Dexamethasone (DEX) is a type of glucocorticoid that has anti-inflammatory properties and is used to treat various diseases such as allergies, autoimmune diseases, and cancer. Recently, it has been found that it could also be useful for treating COVID-19. However, when administered intravenously, the high doses are required to reach a therapeutic effect due to its unfavorable pharmacokinetics (PK). Consequently, the undesirable side effects occur and limit its prescription on a chronic basis. Moreover, repeated dexamethasone injections at high clinical doses can cause a variety of side effects. To address this issue, we have developed a drug delivery system utilizing layered double hydroxide (LDH) as a carrier. DEX was intercalated into the interlayer spaces of LDH using various methods such as co-precipitation and hydrothermal treatment, ion-exchange, exfoliation-reassembling. Based on the X-ray diffraction, molecular spectroscopy and thermogravimetry analyses, the DEX molecules were stabilized in the interlayer spaces of LDH by electrostatic interaction, retaining their functionality and structural integrity. SEM and DLS results showed that the DEX-LDH particles were evenly dispersed with uniform size. We investigated the sustained release properties of DEX under different pH conditions (pH 5.0, pH 6.8, and pH 7.4). 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-437**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Caffeic Acid-Layered Double Hydroxide Nanohybrids for Enhanced Sunscreen Formulations

Dahye Seo, Goeun Choi[1,*], Jin-Ho Choy[2,*]

a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN)b.Department of Chemistry, Dankook University, Korea

[1]*a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN)b.Department of Nanobiomedical Science and BK21 PLUS NBM Global Research Center for Regenerative Medicine, Dankook University, Korea*

[2]*a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN)b.Division of Natural Sciences, the National Academy of Sciences, Seoulc.Department of Pre-medical Course, College of Medicine, Dankook University, Korea*

Caffeic acid (CA), a component derived from plants, has not only antioxidant capabilities but also UV-shielding functionality. However, it exhibits low stability under UV irradiation and exposure to oxygen. To overcome these limitations, the implementation of an effective carrier system for CA is imperative. Layered double hydroxides (LDHs) are well-known for its excellent drug delivery carriers as it is a biocompatible host matrix capable of encapsulating various anionic molecules into its interlayer spaces. In order to improve stability and enhance UV-shielding efficacy, we synthesized CA-LDH nanohybrids by intercalating CA into the interlayer space of LDHs via co-precipitation, ion exchange, and exfoliation-reassembly method. Structural information of CA-LDH nanohybrids was confirmed by XRD and FT-IR analyses, indicating the successful intercalation of CA into the interlayer spaces of LDH. The plate-like morphology and particle size remained consistent after intercalation, as observed through FE-SEM and DLS. The CA contents in CA-LDH nanohybrids were determined at 325 nm using UV-Vis spectroscopy. The UV-shielding performance of CA-LDH nanohybrids surpassed that of pure CA and even commercially available ZnO and TiO2. The CA-LDH nanohybrids also addressed the issue of white cast commonly associated with ZnO and TiO2. The proposed CA-LDH nanohybrids can be applied as a UVA and UVB blocking agent owing to its excellent UVA and UVB(280–400nm) screening property.

Poster Presentation : **MAT.P-438**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Pre-clinical evaluation of injectable photo-thermal agent as triple-negative breast cancer nanomedicine

Sanoj Rejinold Nirichan, Goeun Choi[1], Jin-Ho Choy[2,*]

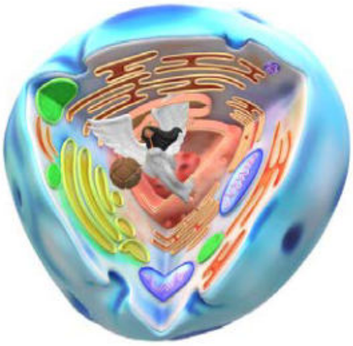
Institute of Tissue Regeneration Engineering (ITREN, a.Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering , Korea

[1]*a. Department of Nanobiomedical Science, b. Institute of Tissue Regeneration Engineering, Dankook University, Korea*

[2]*a. Department of Pre-medical Course, b. Institute of Tissue Regeneration Engineering, Dankook University, Korea*

AbstractTriple-negative breast cancer (TNBC) accounts for ~ 15% of breast cancer incidents and is one of the most lethal cancers for which there is still no proper treatment strategy, mainly due to the lack of three main receptors, HER-2, ER (estrogen receptor), and PR (progesterone receptor), which are commonly found in "normal" breast cancers. Such a challenging situation makes TNBC highly aggressive and untreatable with conventional chemo and immunotherapy. [1] Although there are several advancements in TNBC therapies one of the main advanced therapies is photothermal therapy. However, photo-stability and fast degradation of photo agents are still challenging. For example, IR-780 is one such PTT agent with extremely low aqueous solubility and stability.[2] Here, we rationally designed ~ 200 nm sized IR-780 loaded Zein hybrid NPs and were coated with BSA (BSA-Zein-IR780) making an aqueous soluble photo-thermal agent and tested its suitability as TNBC nanomedicine in Human TNBC cell line (MDA-MB-23) resulting enhanced apoptosis. These preliminary results suggested that the new water-soluble hybrid drug would be advantageous for treating TNBC and other subtypes of breast cancers effectively. Fig. 1. Schematic shows the concept of water-soluble BSA-Zein-IR780 for treating TNBC using photothermal therapy.Keywords: triple-negative breast cancer, IR780, Zein, BSA, In vitro efficacyReferences1. A.M. Karim, J. Eun Kwon, T. Ali, J. Jang, I. Ullah, Y.G. Lee, D.W. Park, J. Park,

J.W. Jeang and S.C. Kang. Biochem Pharmacol. 2023, 212,115545. 2. K. Wang, Y. Zhang, J. Wang, A. Yuan, M. Sun, J. Wu, Y. Hu. Sci Rep. 2016, 6, 27421.



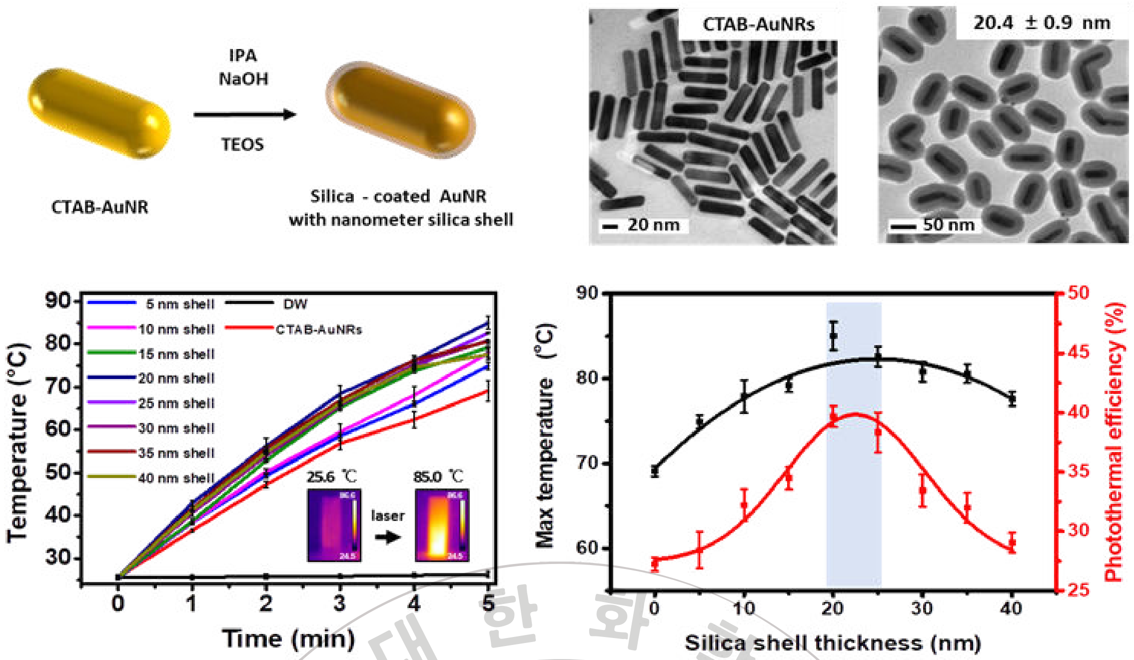
Poster Presentation : **MAT.P-439**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Precise control over the silica shell thickness and finding the optimal thickness for the peak heat diffusion property of AuNR@SiO_2

Wonseok Yang, Dongkwon Lim[1,*]

Korea University, Korea
[1]*KU-KIST Graduate School of Science and Technology, Korea University, Korea*

Gold nanorods (AuNRs), which absorb near-infrared rays and exhibit a photothermal effect, can be coated with silica (SiO2) to improve their effectiveness and stability. Silica-coated AuNRs(AuNR@SiO2) exhibit significantly enhanced photothermal effects and photoacoustic (PA) signal intensities, which is beneficial for various nanophotonic applications in materials science. However, the silica shell thickness for optimum enhancement is not fully understood and is even controversial depending on the physical state of the silica shell. In this study, AuNR@SiO2 with shell thicknesses in the nm range (5 - 40 nm) were synthesized by coating the surface of gold nanorods with SiO2 under selected base and solvent conditions. The photothermal effect efficiency of AuNR@SiO2 according to the thickness of the SiO2 shell was compared and analyzed by irradiating near-infrared rays. The highest photothermal efficiency was shown at a SiO2 shell thickness of 20 nm, which was confirmed to be about 1.45 times higher photothermal efficiency than AuNRs without a SiO2 shell. Along with the thickness, the density of the SiO2 shell also affected the photothermal performance, and the persistence of the photothermal effect was better when the high-density SiO2 shell was formed than when the low-density SiO2 shell was formed. In a cell-based study, AuNRs with a 20 nm silica shell showed the most sensitive photothermal effect for cell death. The results of this robust study can provide conclusive conditions for the optimal silica shell thickness to obtain the highest photothermal effect, which will be useful for the future design of nanomaterials in various fields of application.


IPA
NaOH
TEOS
CTAB-AuNR
Silica - coated AuNR with nanometer silica shell
CTAB-AuNRs
20 nm
20.4 ± 0.9 nm
50 nm
Temperature (°C)
Time (min)
5 nm shell
10 nm shell
15 nm shell
20 nm shell
25 nm shell
30 nm shell
35 nm shell
40 nm shell
DW
CTAB-AuNRs
25.6 ℃
85.0 ℃
laser
Max temperature (°C)
Photothermal efficiency (%)
Silica shell thickness (nm)

Poster Presentation : **MAT.P-440**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

Preparation of Flare-Raman Platform as SERS Probe to Detect Signals by Survivin mRNA Expression in Live Cell

Ju Eun Cho, Dongkwon Lim[1,*]

Korea University, Korea

[1]*KU-KIST Graduate School of Science and Technology, Korea University, Korea*

SiNPs and AuNPs take advantage of being able to functionalize various molecules such as polymers, ligands, and biomolecules. In particular, AuNPs can be used in various fields as a material for effective surface-enhanced Raman spectroscopy (SERS). Meanwhile, survivin mRNA is rarely expressed in normal adult tissues, but is mainly overexpressed in most cancer cells, promoting the growth of tumors.In previous research, detection of mRNA in living cells was possible using a fluorescence-based method. However, fluorescence-based methods are not suitable for real-time experiments due to loss of fluorescence ability due to photobleaching and have a limit of detection (LOD) at the nano-pico molar level (10-10 M). On the other hand, SERS-based method is not limited by photobleaching and have high signal sensitivity at the atto molar level (10-18 M).In this study, SiNPs functionalized with DNA and hybridized with Flare (DNA-Flare-SiNPs) and AuNPs functionalized with DNA of a complementary sequence to Flare (DNA-AuNPs) were prepared, and the fluorescence and SERS signals were compared. By adding survivin mRNA, an increased fluorescence signal was obtained due to the dissociated Flare, and the change in the fluorescence signal was confirmed by capturing the dissociated Flare using DNA-AuNPs.The decrease in fluorescence signal is due to the quenching phenomenon that occurs as the distance to AuNPs approaches through binding to DNA-AuNPs. Due to fluorescence quenching, the Raman signal is turned on, allowing the signal appearing due to the dissociated flare to be detected. These findings suggest the possibility of detecting dynamic changes in survivin mRNA within living cells in real time, which may contribute to cancer diagnosis and cancer treatment research.

Poster Presentation : **MAT.P-441**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Unravelling Active Sites in Additive-Modified Interfacial Architectures for Enhanced Lithium Redox-Driven Nitrogen Reduction to Ammonia

Nguyen Vy

Graduate School of Energy Science and Technology, Chungnam National University, Vietnam

The use of ammonia as an energy carrier and especially fertilizer has triggered numerous interests in developing alternative routes in pursuit of a more decentralized and environmentally friendly approach for ammonia synthesis. Lithium redox-mediated nitrogen reduction is one of the available approaches to electrochemical ammonia production at significant yields under ambient conditions. The significant improvement in the nitrogen reduction reaction (NRR) activity depending on the electrolyte condition suggests a substantial influence of the electrode-electrolyte interphase on the catalytic cycle of NH3 production during Li deposition. However, much remains to be investigated about its systematic analysis. Herein, based on the density functional theory (DFT) calculations, wedemonstrate the critical roles of the surface electrolyte interphase (SEI) layer in enhancing NH3 production from the Lithium redox-mediated NRR by modifying small quantities of additives. In addition, we propose that the well-constructed dual-layer SEI stabilizes the reactive species and thermodynamically favours NRR to NH3 compared with the pristine catalyst surface. Our findings reveal the effect of additives on NRR and provide theoreticalsupport to the reported experimental results in the literature. This investigation offers insights into achieving future high-efficiency NRR system conditions and analyzing electrode SEIs.

Unravelling Active Sites in Additive-Modified Interfacial Architectures for Enhanced Lithium Redox-Driven Nitrogen Reduction to Ammonia

Nguyen Thuy Vy, *, Hyeyoung Shin
Graduate School of Energy Science and Technology, Chungnam National University, Yuseong-gu, Daejeon, 34134, Republic of Korea
*E-mail: 202230129@o.cnu.ac.kr, shinhy@cnu.ac.kr

The use of ammonia as an energy carrier and especially fertilizer has triggered numerous interests in developing alternative routes in pursuit of a more decentralized and environmentally friendly approach for ammonia synthesis. Lithium redox-mediated nitrogen reduction is one of the available approaches to electrochemical ammonia production at significant yields under ambient conditions. The significant improvement in the nitrogen reduction reaction (NRR) activity depending on the electrolyte condition suggests a substantial influence of the electrode-electrolyte interphase on the catalytic cycle of NH_3 production during Li deposition. However, much remains to be investigated about its systematic analysis. Herein, based on the density functional theory (DFT) calculations, we demonstrate the critical roles of the surface electrolyte interphase (SEI) layer in enhancing NH_3 production from the Lithium redox-mediated NRR by modifying small quantities of additives. In addition, we propose that the well-constructed dual-layer SEI stabilizes the reactive species and thermodynamically favours NRR to NH_3 compared with the pristine catalyst surface. Our findings reveal the effect of additives on NRR and provide theoretical support to the reported experimental results in the literature. This investigation offers insights into achieving future high-efficiency NRR system conditions and analyzing electrode SEIs.

Poster Presentation : **MAT.P-442**

Material Chemistry

Exhibition Hall C FRI 11:00~13:00

In silico design of electrocatalysts for enhancing nitrogen reduction reaction

Minh phuong Nguyen

Graduate School of energy science and technology, Chungnam National University, Vietnam

Electrochemical nitrogen reaction (NRR) has been known as a clean and sustainable technology that produces ammonia (NH3) under ambient conditions. Recently, molybdenum-based two-dimensional materials (MoX2, where X = S, Se, and Te) have been widely studied as part of the electrocatalysts for NRR performance due to unique properties favorable for N2 adsorption and activation of Mo element. However, the electrocatalytic activities of these materials are still insufficient, and the atomic-level understanding of the reaction mechanism is lacking. In this study, we present a comprehensive investigation into the electrocatalytic activities of MoX2 compounds doped with transition metal atoms (TM), using density functional theory (DFT) calculations. Our objective is to propose new promising candidates as efficient NRR electrocatalysts by high-throughput screening of 28 TM atoms from the 3d, 4d, and 5d groups embedded in MoX2.

In silico design of electrocatalysts for enhancing nitrogen reduction reaction

Nguyen Minh Phuong,* Hyeyoung Shin
Graduate School of Energy Science and Technology (GEST), Chungnam National University, Yuseong-gu, Daejeon, 34134, Republic of Koreaa
*E-mail: nmphuong947@gmail.com, shinhy@cnu.ac.kr

Electrochemical nitrogen reaction (NRR) has been known as a clean and sustainable technology that produces ammonia (NH_3) under ambient conditions. Recently, molybdenum-based two-dimensional materials (MoX_2, where X = S, Se, and Te) have been widely studied as part of the electrocatalysts for NRR performance due to unique properties favorable for N_2 adsorption and activation of Mo element. However, the electrocatalytic activities of these materials are still insufficient, and the atomic-level understanding of the reaction mechanism is lacking. In this study, we present a comprehensive investigation into the electrocatalytic activities of MoX_2 compounds doped with transition metal atoms (TM), using density functional theory (DFT) calculations. Our objective is to propose new promising candidates as efficient NRR electrocatalysts by high-throughput screening of 28 TM atoms from the 3d, 4d, and 5d groups embedded in MoX_2.

Keywords: nitrogen reduction reaction, electrocatalyst, molybdenum-based two-dimensional materials, density functional theory, high-throughput screening

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **MAT.P-443**
Material Chemistry
Exhibition Hall C FRI 11:00~13:00

Exploring Spinel Cathodes through First-Principle Calculation for Next-Generation Li-ion Battery

Thi Yen Nhi Phan

Graduate School of Energy Science and Technology, Chungnam National University, Vietnam

Co-free spinel structure LiNi0.5Mn1.5O4 (LNMO) has been demonstrated as a promising cathode material for lithium-ion batteries because of its high energy density arising from high operating voltage, superior thermal stability, and high ionic conductivity during electrochemical processes. However, the LNMO spinel cathode experiences a number of problems during LIB operation, including electrolyte degradation as a result of high operating voltage and rapid capacity decay leading to a short battery lifespan, which limits the widespread application and commercialization of this material. Despite intense research efforts that have been focused on the modification of L MO to improve its electrochemical performance, optimizing their compositions remains a challenge. In this work, we perform a computational study using first-principles calculations to evaluate and screen appropriate dopants for the LNMO cathode, focusing on improving their electrochemical performance. The proposed candidates exhibit excellent electrochemical characteristics, higher electronic conductivity, and high stability. These results highlight the promise of using optimized spinel structure materials that can serve as cost-effective and high-performance cathodes for lithiumion batteries.

Exploring Spinel Cathodes through First-Principle Calculation for Next-Generation Li-ion Battery

Phan Thi Yen Nhi*, Truong Ba Tai, Hyeyoung Shin
Graduated School of Energy Science and Technology, Chungnam National University, Yuseong-gu, Daejeon, 34134, Republic of Korea
*E-mail: ptynhi.ctu@gmail.com, shinhy@cnu.ac.kr

Co-free spinel structure $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) has been demonstrated as a promising cathode material for lithium-ion batteries because of its high energy density arising from high operating voltage, superior thermal stability, and high ionic conductivity during electrochemical processes. However, the LNMO spinel cathode experiences a number of problems during LIB operation, including electrolyte degradation as a result of high operating voltage and rapid capacity decay leading to a short battery lifespan, which limits the widespread application and commercialization of this material. Despite intense research efforts that have been focused on the modification of LNMO to improve its electrochemical performance, optimizing their compositions remains a challenge. In this work, we perform a computational study using first-principles calculations to evaluate and screen appropriate dopants for the LNMO cathode, focusing on improving their electrochemical performance. The proposed candidates exhibit excellent electrochemical characteristics, higher electronic conductivity, and high stability. These results highlight the promise of using optimized spinel structure materials that can serve as cost-effective and high-performance cathodes for lithium-ion batteries.

Poster Presentation : **ELEC.P-380**

Electrochemistry

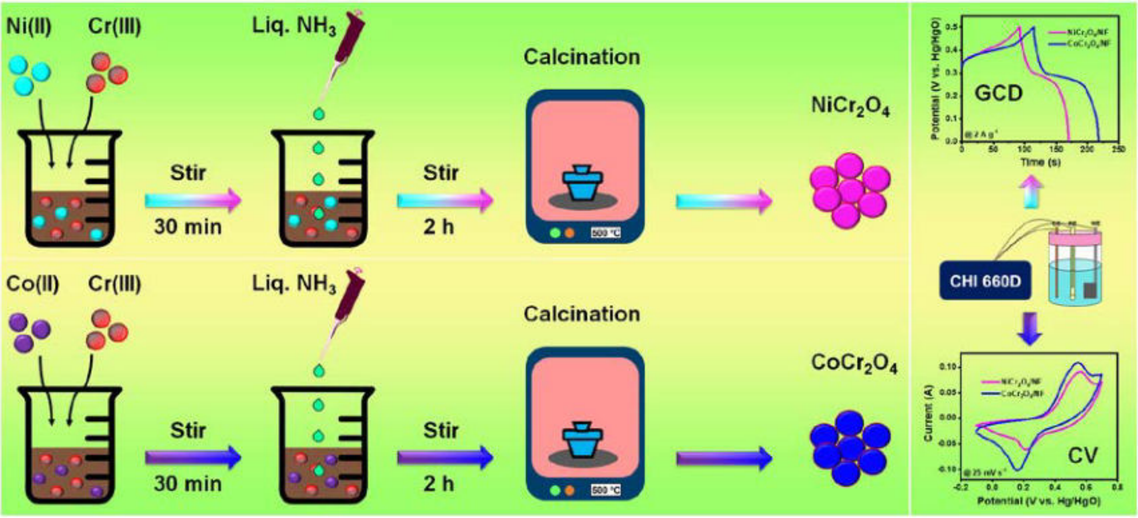
Exhibition Hall C THU 11:00~13:00

Fabrication of Spinel MCr2O4 (M = Ni and Co) Nanostructures as Positive Electrode Materials for High-Performance Supercapacitors

Venkatachalam Vinothkumar, Tae Hyun Kim*

Department of Chemistry, Soonchunhyang University, Korea

Nanostructured spinel transition metal oxides (TMOs) have been considered promising and reliable electrode materials for energy storage devices, especially supercapacitors, owing to their unique structural features and excellent electrochemical properties. Herein, we developed spinel MCr2O4 (M = Ni and Co) nanostructures by the facile and straightforward coprecipitation method and evaluated as efficient electrode materials for high-performance supercapacitors. Due to its more electroactive sites, increased surface area, better electrical conductivity, and synergistic effects of binary metals, the fabricated CoCr2O4/NF electrode exhibits a higher specific capacitance of 550 F g–1 at the current density of 1 A g–1 than the NiCr2O4/NF electrode (442 F g–1 at 1 A g–1). Moreover, the CoCr2O4/NF electrode presents excellent cyclic stability of 94.15% capacitance retention compared with NiCr2O4/NF electrode (90.82%) after 5000 cycles at 10 A g–1. In addition, the asymmetric supercapacitor (CoCr2O4/NF//AC/NF) assembled with CoCr2O4/NF positive electrode and activated carbon (AC/NF) negative electrode delivers a good specific capacitance of 114.12 F g–1 (at 1 A g–1), considerable cyclability of 89.4% (over 5000 cycles at 10 A g–1), and maximum energy density of 45.80 W h kg–1 at a power density of 849.9 W kg–1. Therefore, this study offers a new path for the fabrication of high-performance spinel nanomaterials for supercapacitors.


Ni(II)
Cr(III)
Liq. NH$_3$
Stir
30 min
Stir
2 h
Calcination
500 °C
NiCr$_2$O$_4$
Co(II)
Cr(III)
Liq. NH$_3$
Stir
30 min
Stir
2 h
Calcination
500 °C
CoCr$_2$O$_4$
GCD
NiCr$_2$O$_4$/NF
CoCr$_2$O$_4$/NF
@2 A g^{-1}
Potential (V vs. Hg/HgO)
Time (s)
0
50
100
150
200
250
0.0
0.1
0.2
0.3
0.4
0.5
CHI 660D
CV
NiCr$_2$O$_4$/NF
CoCr$_2$O$_4$/NF
@25 mV s^{-1}
Current (A)
Potential (V vs. Hg/HgO)
-0.2
0.0
0.2
0.4
0.6
0.8
-0.10
-0.05
0.00
0.05
0.10

Poster Presentation : **ELEC.P-381**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Application of Deep Learnging to Analysis of Electrochemical Impedance Spectra

Byoung-Yong Chang

Department of Chemistry, Pukyong National University, Korea

The field of electrochemical impedance spectroscopy has witnessed recent innovations that enable the gathering of extensive spectral data in a fraction of the time once required. However, current analytical methods struggle to keep up with the rapid evolution of the instrumental technologies, creating a need for more efficient processing. This study presents a solution to this issue by introducing a new method that employs deep learning techniques for the analysis of electrochemical impedance spectra, specifically upon varying potential. Through the utilization of an auto-encoder, a form of deep neural network, the impedance data is processed and encoded into two-dimensional latent vectors. These vectors encapsulate critical information representing the electrochemical processes that alter in reaction to changes in electrode potential, encompassing aspects like charge transfer, mass transfer, and electric double-layer charging. When decoded, the latent vectors generate impedance spectra of a higher quality. The successful application of this method offers a groundbreaking proof of concept for the automated analysis of electrochemical impedance spectra through the utilization of machine learning techniques.

Poster Presentation : **ELEC.P-382**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Wash-Free Photoelectrochemical DNA Detection Based onPhotoredox Catalysis Combined with Electroreduction and LightBlocking by Magnetic Microparticles

Jihyeon Kim, Haesik Yang[1,*]

Department of chemistry, Pusan National University, Korea

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

To obtain a sensitive, wash-free photoelectrochemical biosensor based on electron mediation between an electrode and a photoredox catalyst (PC) label, unavoidable O2-related reactions should have no effect or be beneficial, and the rate of electron mediation should depend on the distance between the PC label and electrode. A wash-free photoelectrochemical biosensor that (i) combines photoredox catalysis of a PC label with electrochemical reduction of an electron mediator, and (ii) uses a light-blocking multilayer of magnetic microparticles was developed. O2 participates as an electron acceptor in photoredox catalysis; thus, increasing rather than decreasing the electrochemical signal. Upon photoirradiation from the opposite side of a transparent indium tin oxide (ITO) electrode in contact with the solution, the light intensity in the solution is sharply decreased by the light-blocking multilayer, which increases the contribution of affinity-bound PC labels on the ITO electrode to the electrochemical signal compared to that of unbound PC labels in solution. Utilizing eosin Y (EY2−) and Fe(CN)64− as the PC and electron mediator (i.e., electron donor), respectively, enabled rapid redox cycling based on photoredox catalysis combined with electroreduction. The cathodic charge is mainly related to electron transfer from Fe(CN)64− to excited EY2−(Type I photosensitization), rather than energy transfer from excited EY2− to O2, which generates 1O2 (Type II photosensitization). The developed detection scheme was applied to wash-free detection of a model target DNA. Detection limits of ~200 pM were obtained in both phosphate-buffered saline and serum without washing. The developed scheme enables simple photoelectrochemical detection.

Poster Presentation : **ELEC.P-383**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Sensitive Affinity-Based Biosensor Using the Autocatalytic Activation of Trypsinogen Mutant by Trypsin with Low Self-activation

Seonhwa Park, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Propagating catalysis cascades that enable high signal amplification are not common in affinity-based biosensors owing to the limited number of catalytically activable catalytic materials available. In this regard, enzymatically activable proenzymes are well suited to propagating catalysis cascades. Here, we report that a self-propagating autocatalytic reaction based on the activation of trypsinogen by trypsin facilitates high signal amplification and a low detection limit for prostate-specific antigen (PSA). Trypsin, which is used as a catalytic label in a sandwich-type immunosensor, converts trypsinogen into trypsin; the generated trypsin then further converts trypsinogen into trypsin. The autocatalytically produced trypsin proteolytically cleaves the peptide bond of a trypsin substrate, resulting in the liberation of electrochemically active 4-aminophenol (AP). The electrochemical oxidation of AP at a modified indium tin oxide (ITO) electrode induces electrochemical–chemical redox cycling involving the ITO electrode, AP, and a reductant. The triple combination of autocatalytic activation, proteolytic cleavage, and redox cycling results in a high electrochemical signal level. A commercially available trypsinogen mutant minimizes the autoactivation of trypsinogen by trypsinogen, thereby providing a low electrochemical background level. The detection limit for PSA obtained using a trypsin label and trypsinogen (~7 pg/mL) is lower than that obtained using a trypsin label alone (~100 pg/mL). This study demonstrated that autocatalytically activating a proenzyme is a very useful method for highly amplifying signals.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-384**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Rapid nanocatalytic reaction using antibody-conjugated gold nanoparticles for sensitive detection of parathyroid hormone

Gyeongho Kim, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Biomolecule-conjugated metal nanoparticles (NPs) have been primarily used as colorimetric labels in affinity-based bioassays for point-of-care testing. A facile electrochemical detection scheme using a rapid nanocatalytic reaction of a metal NP label is required to achieve more quantitative and sensitive point-of-care testing. Moreover, all the involved components should be stable in their dried form and solution. In this presentation, the development of a stable component set enabling rapid and simple nanocatalytic reactions and its application to the sensitive detection of parathyroid hormone (PTH) are reported. The component set consists of an indium–tin oxide (ITO) electrode, ferrocenemethanol (FcMeOH), antibody-conjugated Au NPs, and ammonia borane (AB). Despite being a strong reducing agent, AB is selected because it is stable in its dried form and solution. The slow direct reaction between FcMeOH+ and AB provides a low electrochemical background, and the rapid nanocatalytic reaction allows for a high electrochemical signal. Under optimal conditions, PTH could be quantified in a wide range of concentrations in artificial serum, with a detection limit of ~0.5 pg/mL. Clinical validation of the developed PTH immunosensor using real serum samples indicates that this novel electrochemical detection scheme is promising for quantitative and sensitive immunoassays for point-of-care testing.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-385**

Electrochemistry

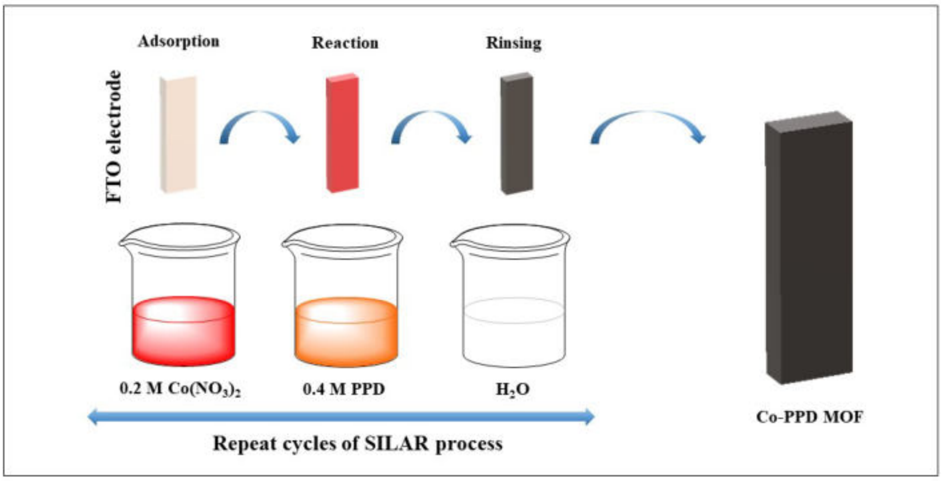
Exhibition Hall C THU 11:00~13:00

Facile Synthesis of Co3O4 Thin Films and Subsequent Conversion to Cobalt Chalcogenides: Application to Supercapacitors

<u>Seonghwan Yu</u>, Tae Wan Park, Soo Yeon Kim, Noseung Myung[*]

Department of Applied Chemistry, Konkuk University, Korea

A strategy for the synthesis of Co3O4 films and their subsequent conversion to the corresponding chalcogenides was developed. Co-PPD was prepared by a SILAR method using Co2+ cation precursor and a p-phenylendiamine anion precursor at room temperature. As-prepared Co-PPD MOF films were converted into Co3O4 after heat treatment at 450 ℃ under air. The MOF-derived Co3O4 films were then employed as a sacrificial template to fabricate cobalt chalcogenides films via anion exchange with chalcogenides medium. All films were characterized by a variety of experimental techniques including FT-IR, FESEM, XRD, and XPS. Thus, Co3O4/Co-X (X = S or Se) core shell films showed improved capacitive behavior compared with Co3O4 film.


Adsorption
Reaction
Rinsing
FTO electrode
0.2 M $Co(NO_3)_2$
0.4 M PPD
H_2O
Repeat cycles of SILAR process
Co-PPD MOF

Poster Presentation : **ELEC.P-386**

Electrochemistry

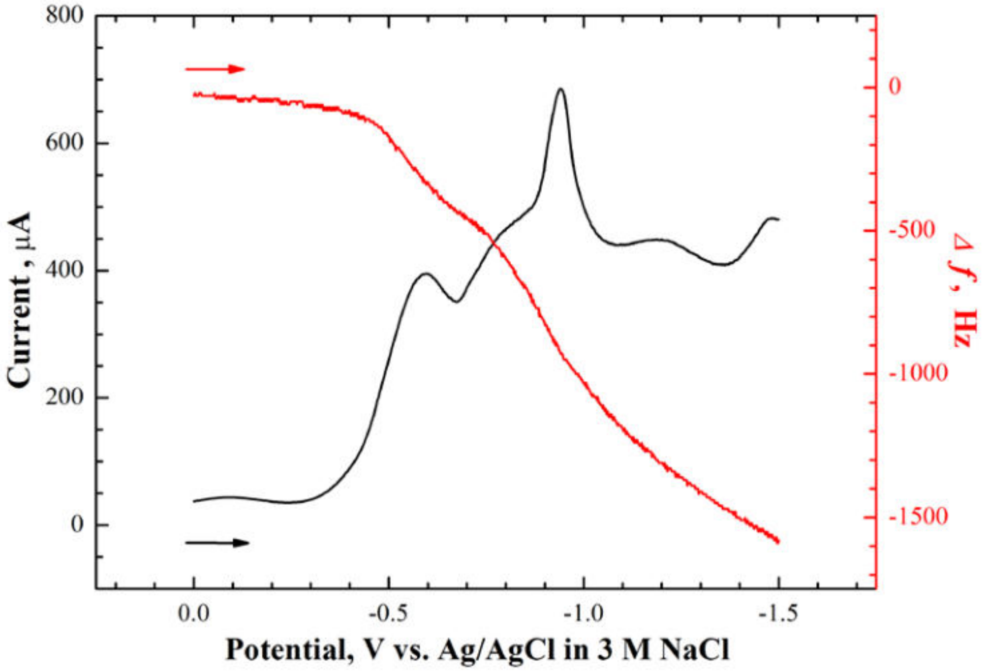
Exhibition Hall C THU 11:00~13:00

Electrodeposition of Nickel Selenide Thin Films: An EQCM Study

Soo Yeon Kim, Noseung Myung*

Department of Applied Chemistry, Konkuk University, Korea

The mechanism of electrodeposition of nickel selenide thin films was investigated by the combined application of linear sweep voltammetry (LSV) and electrochemical quartz crystal microgravimetry (EQCM) on Au-coated quartz electrodes. Nickel selenide films were electrodeposited on the Au surface from 0.1 M Na2SO4 electrolyte solution containing 10 mM NiCl2 and 10 mM SeO2 by linear sweep voltammetry. Five cathodic waves were observed during the linear scans and the reactions corresponding to these waves were investigated with LSV and EQCM. As a result, XRD study showed that as prepared films are Ni3Se2.


800
600
400
200
0
Current , μA
0
-500
-1000
-1500
Δ f , Hz
0.0
-0.5
-1.0
-1.5
Potential, V vs. Ag/AgCl in 3 M NaCl

Poster Presentation : **ELEC.P-387**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Utilizing Perovskite BaIrO3 Nanofibers for Potentiometric pH Sensing Applications

Subin Choi, Hee Ah Oh[1], Youngmi Lee[2,*], Myung Hwa Kim[2]

Ewha Womans University, Korea

[1]*Deparment of Chemistry & Nanoscience, Ewha Womans University, Korea*

[2]*Department of Chemistry & Nanoscience, Ewha Womans University, Korea*

The extensive implications in domains such as health assessment have generated substantial demand for precise pH measurements. Glass electrodes in pH sensing has been driven by their commendable attributes encompassing sensitivity and selectivity. Nevertheless, these electrodes are not immune to specific challenges, notably vulnerability to alkaline errors. As a result, a proactive pursuit of novel materials to amplify pH electrode performance has been undertaken. Within this framework, iridium oxide (IrOx) has emerged as a promising alternative, affording merits such as the capacity to detect an extensive pH spectrum and diminished susceptibility to chemical interference. Nonetheless, prudent consideration of the economic dimension is crucial, necessitating endeavors to curtail the usage of noble metals (e.g., Ir) while concurrently augmenting performance.In this work, we introduce perovskite BaIrO3 nanofibers as an enhanced potentiometric pH sensing material in a wide pH range upto extremely basic conditions. BaIrO3 nanofibers were synthesized via electrospinning and calcination processes. The morphology of BaIrO3 nanofibers was measured by field-emission scanning electron microscopy (FE-SEM). The physical property of BaIrO3 nanofibers was analyzed by X-ray diffraction (XRD). The pH value was determined by the open-circuit potentials in various buffer solutions such as commercial pH buffer solutions and universal buffer solutions. Acid-base titration measurements were also conducted to determine the response time of BaIrO3 nanofibers. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984 and NRF-2023R1A2C2003187).


사단법인
대한화학회
KOREAN CHEMICAL SOCIETY

Poster Presentation : **ELEC.P-388**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Reliable bi-functional Ni-Pi/TiO2 integration enables stable n-GaAs photoanode for water oxidation under alkaline condition

Maheswari Arunachalam, Soon Hyung Kang[1,*]

Department of Chemistry Education, Chonnam National University, Korea

[1]*Department of Chemical Education, Chonnam National University, Korea*

Hydrogen is one of the most widely used essential chemicals worldwide, and it is also employed in the production of many other chemicals, especially carbon-free energy fuels produced via photoelectrochemical water splitting. At present, gallium arsenide represents the most efficient photoanode material for PEC water oxidation, but it is known to either be anodically photocorroded or photopassivated by native metal oxides in the competitive reaction, limiting efficiency and stability. Here, we report chemically etched GaAs that is decorated with thin titanium dioxide (~30-nm-thick, crystalline) surface passivation layer along with nickelphosphate cocatalyst as a surface hole-sink layer. The integration of Ni-Pi bifunctional co-catalyst results in a highly efficient GaAs electrode with a ~100 mV cathodic shift of the onset potential. In this work, the electrode also has enhanced photostability under 110-h testing for PEC water oxidation at a steady current density Jph > 25 mA·cm−2. The Et-GaAs/TiO2/Ni-Pi ‖ Ni-Pi tandem configuration results in the best unassisted bias-free water splitting device with the highest Jph (~7.6 mA·cm−2) and a stable solar-to-hydrogen conversion efficiency of 9.5%.

Poster Presentation : **ELEC.P-389**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Study of PEC performance of silica photocathode protected by TiN layer

Soon Hyung Kang*, Suzan Sayed[1]

Department of Chemical Education, Chonnam National University, Korea

[1]*Chemical Engineering, Chonnam National University, Egypt*

Burning of fossil flues and emission of greenhouse gases caused global warming, widespread a rapid changes in atmosphere that impacts losses and damages on nature and people. That triggered the need of clean renewable and sustainable energy sources. H_2 is a carbon-free source with a high energy storage density, and its generation through photoelectrochemical (PEC) water splitting using solar harvesting is the most attractive strategy to address these environmental, energy demand, and supply issues.1,2 Recently, Transition metal Nitride has an enormous interest in various applications due to its unique physical properties such as: high conductivity, corrosion resistance and extreme hardness. Here in we report the deposition of polycrystaline thin film TiN by DC Magnetron sputtering on Si photocathode as a protective layer in acidic media. The rocksalt nitride (TiN) film demonstrated prevention of Si degradation with improvement in the photocurrent density and long-term stability under simulated 1.5AMG illumination.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ELEC.P-390**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Detection of Gel Particles via Nanoimpact

Haneul Park, Jun Hui Park[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

In this study, we have developed a system to detect single hydrogel particles in an aqueous solution using a patterned electrode. The stability of gel particles is based on the oxidation state of metal ions. To create stable gel particles, we used a type of ‘hard’ metal cation that promotes the formation of cross-linked hydrogels. We found that when a single gel particle collides with the electrode, it partially blocks the flow of current due to its adsorption properties, such as its contact area. The collisions were recorded using amperometric current-time (I-t) measurements, which revealed a sudden change in the electrical current when the electrode surface was blocked. The size distribution of the gel particles obtained from the electrochemical signals matched well with the dynamic light scattering (DLS) result. By studying these collision events, we can obtain a better understanding of hydrogel particle properties.

Poster Presentation : **ELEC.P-391**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

MoS2/MnMoO4@Ti nanocomposite electrocatalyst for efficient hydrogen evolution reaction

<u>Jyoti Badiger</u>, Soon Hyung Kang[1,*]

Photonic Engineering, Chonnam National University, India

[1]*Department of Chemical Education, Chonnam National University, Korea*

Nowadays, it is very important to produce low cost, environmentally friendly and cheaper electrocatalysts for electrocatalytic hydrogen evolution reaction with superior characteristics [1]. Considering this approach, MoS2 based catalysts have been used widely due to their electrochemical catalytic activity, low cost, most promising and high efficiency alternative to Pt for HER [2] but it suffers from low conductivity and limited active edges [3]. To overcome this problem, we report MoS2/MnMoO4 nanocomposite by varying ratios of Mo:Mn using one step hydrothermal reaction which gives improved catalytic activities. In particular, MoS2/MnMoO4 (Mo:Mn = 1:2.5) has an lower overpotential of -153 mV to drive current density of 10 mA/cm-2 than other ratios of Mo:Mn and also gives excellent stability upto 100 hr towards HER in acidic medium. According to the analysis, MoS2 nanosheets combined with MnMoO4 rods are more electrochemically active than either alone. The combined effect of manganese and molybdenum ions from MnMoO4 produces more redox chemistry reactions that can help expose more MoS2 nano sheets active sites allowing commercial electrocatalysts to be designed.

$MoS_2/MnMoO_4$@Ti nanocomposite electrocatalyst for efficient hydrogen evolution reaction

Jyoti Badiger [1] and Soon Hyung Kang [2, *]

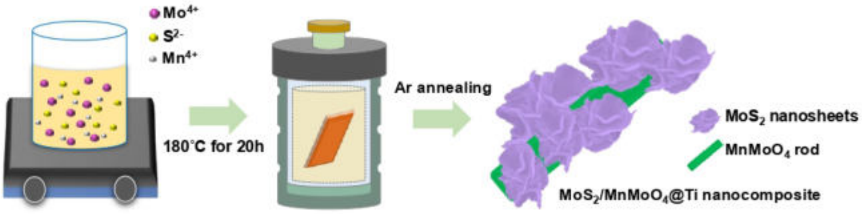
[1] *Department of Interdisciplinary Program for Photonic Engineering, Chonnam National University, Gwangju 61186, Republic of Korea.*

[2] *Department of Chemistry Education and Optoelectronic Convergence Research Center, Chonnam National University, Gwangju 61186, Republic of Korea.*

* *Presenting author (jyotibadiger@gmail.com)*

** *Corresponding author (skang@jnu.ac.kr)*

Nowadays, it is very important to produce low cost, environmentally friendly and cheaper electrocatalysts for electrocatalytic hydrogen evolution reaction with superior characteristics [1]. Considering this approach, MoS_2 based catalysts have been used widely due to their electrochemical catalytic activity, low cost, most promising and high efficiency alternative to Pt for HER [2] but it suffers from low conductivity and limited active edges [3]. To overcome this problem, we report $MoS_2/MnMoO_4$ nanocomposite by varying ratios of Mo:Mn using one step hydrothermal reaction which gives improved catalytic activities. In particular, $MoS_2/MnMoO_4$ (Mo:Mn = 1:2.5) has an lower overpotential of -153 mV to drive current density of 10 mA/cm^{-2} than other ratios of Mo:Mn and also gives excellent stability upto 100 hr towards HER in acidic medium. According to the analysis, MoS_2 nanosheets combined with $MnMoO_4$ rods are more electrochemically active than either alone. The combined effect of manganese and molybdenum ions from $MnMoO_4$ produces more redox chemistry reactions that can help expose more MoS_2 nano sheets active sites allowing commercial electrocatalysts to be designed.



Scheme 1. Schematic illustration of the synthesis process for the $MoS_2/MnMoO_4$@Ti nanocomposite.

Reference: 1. X. Wang, H. Zhou, D. Zhang, M. Pi, J. Feng, S. Chen, Journal of power sources,387 (2018) 1-8.
2. G. Wang, G. Zhang, X. Ke, X. Chen, X. Chen, Y. Wang, G. Huang, J. Dong, S. Chu, M. Sui, Small,18 (2022).
3. Y. Wan, Z. Zhang, X. Xu, Z. Zhang, P. Li, X. Fang, K. Zhang, K. Yuan, K. Liu, G. Ran, Y. Li, Y. Ye, L. Dai,Nano energy,51 (2018) 786-792.

Poster Presentation : **ELEC.P-392**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

N Doping ZnO Electrocatalysts Towards Electrochemical CO2 Reduction

Soon Hyung Kang*, Rohini Kanase[1]

Department of Chemical Education, Chonnam National University, Korea

[1]*Chonnam National University, India*

The discovery of efficient, selective, and stable electrocatalysts can be a main key point to producing large-scale chemical fuels via electrochemical CO2 reduction (ECR). In this study, an earth-abundant and nontoxic ZnO-based electrocatalyst was developed for use in gas-diffusion electrodes, and the effect of nitrogen (N) doping on the ECR activity of ZnO electrocatalysts was investigated. Initially, a ZnO nanosheet was prepared via the hydrothermal method, and nitridation was performed at different times to control the N-doping content. With an increase in the N-doping content, the morphological properties of the nanosheet changed significantly, namely the 2D nanosheets transformed into irregular shaped nanoparticles. Furthermore, the ECR performance of ZnO electrocatalysts with different N-doping content was determined. While the ECR activity increased after a small amount of N doping, it decreased for higher N doping content. Among them, the N:ZnO-1h electrocatalysts were investigated and showed the best CO selectivity, with a Faradaic efficiency (FECO) of 92% at -0.73 V vs. reversible hydrogen electrode, which was greater than that of an undoped ZnO electrocatalyst (FECO of 67% at -0.78 V). N:ZnO-1h electrocatalyst exhibited outstanding durability for 16 h, with a partial current density of -92.1 mA·cm-2. This improvement of the CO selectivity of N:ZnO-1h electrocatalysts can be explained by i) the higher adsorption capacity resulting from the N-doping of ZnO, ii) the reaction between N atoms and the O atoms of ZnO, stabilizing the intermediates formed during ECR and iii) the interfacial charge transfer reaction increasing the electron transfer rate.

N Doping ZnO Electrocatalysts Towards Electrochemical CO_2 Reduction

* Rohini Kanase[1], and ** Soon Hyung Kang[3]
[1] *Department of Interdisciplinary Program for Photonic Engineering, Chonnam National University, Gwangju 61186, South Korea*
[2] *Department of Chemistry education, Chonnam National University, Gwangju 61186, South Korea*

** Presenting author (rohinikanase@gmail.com)*
*** Corresponding author (skang@jnu.ac.kr)*

The discovery of efficient, selective, and stable electrocatalysts can be a main key point to producing large-scale chemical fuels via electrochemical CO_2 reduction (ECR). In this study, an earth-abundant and nontoxic ZnO-based electrocatalyst was developed for use in gas-diffusion electrodes, and the effect of nitrogen (N) doping on the ECR activity of ZnO electrocatalysts was investigated. Initially, a ZnO nanosheet was prepared via the hydrothermal method, and nitridation was performed at different times to control the N-doping content. With an increase in the N-doping content, the morphological properties of the nanosheet changed significantly, namely the 2D nanosheets transformed into irregular shaped nanoparticles. Furthermore, the ECR performance of ZnO electrocatalysts with different N-doping content was determined. While the ECR activity increased after a small amount of N doping, it decreased for higher N doping content. Among them, the N:ZnO-1h electrocatalysts were investigated and showed the best CO selectivity, with a Faradaic efficiency (FE_{CO}) of 92% at -0.73 V vs. reversible hydrogen electrode, which was greater than that of an undoped ZnO electrocatalyst (FE_{CO} of 67% at -0.78 V). N:ZnO-1h electrocatalyst exhibited outstanding durability for 16 h, with a partial current density of -92.1 $mA \cdot cm^{-2}$. This improvement of the CO selectivity of N:ZnO-1h electrocatalysts can be explained by i) the higher adsorption capacity resulting from the N-doping of ZnO, ii) the reaction between N atoms and the O atoms of ZnO, stabilizing the intermediates formed during ECR and iii) the interfacial charge transfer reaction increasing the electron transfer rate.

Poster Presentation : **ELEC.P-393**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Investigating Tin Oxide Catalysts for Selective Electrochemical Reduction of Carbon Dioxide into Formate

Hyeon Beom Cho, Joon Yong Park, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

The electrochemical reduction of carbon dioxide (CO_2RR) is a promising and eco-friendly approach for producing feasible energy sources, while simultaneously mitigating CO_2 emissions and climate problems. Among heterogeneous metal-based materials, Sn-based catalysts have been found to exhibit relatively high selectivity for producing formate from CO_2 via a two-electron transfer pathway, which is highly desirable for industrial feedstock. In addition, Sn-based catalysts are attractive due to their low cost, low toxicity, and their appropriate adsorption strength for specific intermediates. In this study, the SnO catalyst as an electrochemical catalyst was performed in an H-type cell to measure the efficiency of CO_2RR. It exhibited high activity and selectivity towards formate, the desirable Faradaic efficiencies of over 80% in a wide potential window from −1.16 V to −1.56 V (vs. RHE). To understand the high formate selectivity of the catalyst, we investigated the interaction between Sn and O sites for CO_2RR, starting with comparative XRD peak analysis according to each reaction process. And, to achieve higher selectivity than this, the metal photodeposition was also performed. These results suggest that the formation of Sn-O-CO_2 intermediate played a crucial role in the selective production of formate and emphasized the possibility of SnO nanoparticles as an efficient electrocatalyst for CO_2RR.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-394**

Electrochemistry

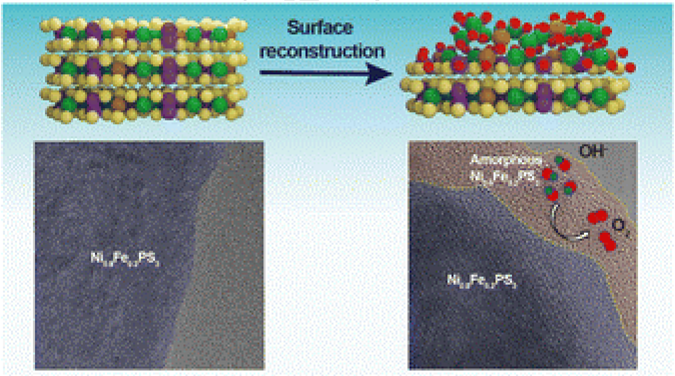
Exhibition Hall C THU 11:00~13:00

Unraveling the surface self-reconstruction of Fe-doped Ni-thiophosphate for efficient oxygen evolution reaction

Yo Seob Won

Chemistry, Sungkyunkwan University, Korea

Surface self-reconstruction of oxygen evolution reaction (OER) electrocatalysts generally occurs during the electrochemical activation process. Herein, we study the surface self-reconstruction of a 2D layered Fe-doped Ni-thiophosphate (NixFe1−xPS3) nanosheet. The role of Fe in the surface self-reconstruction of NiPS3 during the OER is investigated by using an in situ Raman analysis. Formation of amorphous metal/non-metal oxide layers on the surface of NixFe1−xPS3 can efficiently act as the ultimate catalytic center for the OER.



Poster Presentation : **ELEC.P-395**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Electrochemical monitoring of thermodynamics/kinetics at nanoscale interface of a liquid droplet

Hyeongkwon Moon, Jun Hui Park[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Single-entity has been electrochemically monitored to individually study of its characteristics, such as metal nanoparticles, biomaterials, nanobubbles, liquid droplets, and vesicles. Herein, we report the electrochemical monitoring of attoliters of water droplets in an organic medium by the electrolysis of an extracted redox species from the continuous phase upon collisional events on an ultramicroelectrode. To obtain information about a redox-free water droplet in an organic solvent, redox species with certain concentrations need to be contained inside it. The redox species inside the droplet were delivered by a partitioning equilibrium between the organic phase and the water droplets. The mass transfer of the redox species from the surrounding organic phase to the droplet is very fast because of the radial diffusion, which resultantly establishes the equilibrium. Upon the collisional contact between the droplet and the electrode, the extracted redox species in the water droplets were selectively electrolyzed, even though the redox species in the organic continuous phase remained unreacted because of the different solvent environments. The electrolysis of the redox species in the droplets, where the concentration is determined by the equilibrium constant of the redox species in water/oil, can be used to estimate the size of single water droplets in an organic solution.

Poster Presentation : **ELEC.P-396**
Electrochemistry
Exhibition Hall C THU 11:00~13:00

Synergistic Effects of Green Additives on Melt Electrospinning of Biodegradable Polymer

Yun Hyeong Lee, Jee Woo Kim[1], Byung-Kwon Kim[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1] *분석화학, Ewha Womans University, Korea*

Biodegradable polymer (BP) is recognized as an immensely attractive class of materials, appreciated for their favorable physical characteristics, renewability, compatibility with living systems, and capacity to undergo natural degradation. As a result, BPs have found versatile applications spanning a range of sectors, including pharmaceuticals, medical devices, food packaging, environmental preservation, textiles, and the apparel industry.[1]To enhance the processability of BP in melt electrospinning, we conducted additive experiments using gallic acid (GA) and quercetin (QC) as selected additives based on their promising performance in prior additive experiments for electrospinning.[2] In this study, we conducted experiments involving naturally derived compound additives. Specifically, we focused on comparing the electrical conductivity and viscosity at identical concentrations. The investigation aimed to evaluate the impact of these additives on both conductivity and viscosity, with the goal of approximately confirming potential synergies or discrepancies.Our findings contribute to the understanding of how these naturally occurring compounds influence the electrical and rheological properties of biodegradable polymer, providing valuable insights for applications in various fields where these properties play a critical role.

Poster Presentation : **ELEC.P-397**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Size Control of BaTaO2N Crystals for Efficient Solar-Driven Photoelectrochemical(PEC) Water Splitting

<u>Minseok Ki</u>, Jeongsuk Seo[1,*]

Department of Chemsitry, Chonnam National University, Korea

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

To combat global warming resulting from excessive fossil fuel use, producing hydrogen energy is a highly effective approach. Metal oxynitrides AB(O,N)3 (A = Ba, Sr, B = Ta, Nb) with a perovskite structure possess an appropriate bandgap absorbing visible light and position for facilitating water splitting to produce hydrogen. BaTaO2N is capable of absorbing visible light up to 660 nm(Eg = 1.9 eV).Recent research highlights a significant enhancement in the photocatalytic activity of SrTiO3 crystals in a powder suspension system. This boost was achieved by selectively depositing a cocatalyst such as CoOx on both electron and hole-rich facets of the semiconductor [1]. This approach improves charge separation, reducing recombination, and accelerates the photoreaction. Similarly, BaTaO2N crystals synthesized via KCl flux-assisted nitridation exclusively exhibit {100}- and {110}- oriented facets [2]. By selectively depositing cocatalysts onto these facets by photoelectrodeposition, an increase in PEC water splitting activity may be observed.Our study aims to modulate the crystal size of facet-engineered BaTaO2N through KCl flux-assisted nitridation to improve PEC water splitting. When synthesized at 1123 K with a KCl flux of 10 mol%, $BaTaO_2$ N crystals had an approximate size of 200 nm. The synthesis parameters such as concentration of KCl, nitridation temperature, and so on were investigated to obtain larger size of BaTaO2N leading to fully harvest long-wavelength photons. In a poster session we will discuss the effect of synthesis temperature and the concentration of KCl flux on the surface properties of BaTaO2N, as well as its PEC water splitting activity.[1] Mu, L et al. Energy Environ Sci. 2016, 9, 2463-2469[2] Ying, L et al. Mater. Interfaces. 2019, 22264-22271

Poster Presentation : **ELEC.P-398**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Visible-light-driven Seawater Splitting over LaTiO2N Crystals Prepared by Nitridation of Layered Perovskite BaLa4Ti4O15

Thanh Tam Thi Tran, Jeongsuk Seo[*]

Department of Chemistry, Chonnam National University, Korea

A perovskite oxynitride LaTiO2N is a promising semiconductor with an ideal bandgap energy of 2.1 eV which enables the absorption of visible light up to 600 nm. [1] In previous reports, LaTiO2N was synthesized by ammonolysis of the La2Ti2O7 [2,3], causing large defects such as reduced Ti3+ and anion vacancies. [4] Therefore, the LaTiO2N with low defect density must be essentially synthesized to suppress trapping and recombination of photoexcited carriers, thus accelerating the PEC water splitting activity. In this study, we report the synthesis of perovskite LaTiO2N via nitridation of the highly crystalline BaLa4Ti4O15 crystals prepared by flux-assisted calcination for seawater splitting under AM 1.5G sunlight illumination. According to the X-ray diffraction results, a layered perovskite oxide BaLa4Ti4O15 was completely transformed to perovskite oxynitride LaTiO2N. Moreover, UV-visible diffusion reflectance spectroscopy indicated that the light absorption edge of BaLa4Ti4O15 at 320 nm extended to that of LaTiO2N at 620 nm due to the partial replacement of O2- by N3- in band structure of the oxide during nitridation. The LaTiO2N photoanode was fabricated by a spin coating method. After loading with CoOx cocatalyst, the LaTiO2N photoanode showed PEC seawater splitting activity approximately four times greater than that prepared from La2Ti2O7 for comparison in 0.2 M KPi and 0.5 M NaCl electrolyte at pH 6.4 under AM 1.5 sunlight illumination. The physical properties and the corresponding PEC activities of the prepared LaTiO2N photoanodes will be discussed in a poster presentation. Reference:[1] Angew. Chem. Int. Ed., 2018, 57, 8396-8415[2] J. Phys. Chem. A 2002, 106, 6750–6753[3] J. Am. Chem. Soc. 2012, 134, 8348–8351 [4] Nano Lett. 2014, 14, 1038 – 1041

Poster Presentation : **ELEC.P-399**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Electrochemical Detection of Silver Nanoparticle Collisions on a Gold Electrode

Yerin Bang, Soongyu Han, Sieun Kim, Subin Kim, Seung-Ryong Kwon[*]

Department of Chemistry, Gyeongsang National University, Korea

Silver nanoparticles (AgNPs) are widely used for many applications including medicine, electronics, antibacterial, food, textiles, and energy conversions. The size of AgNPs greatly affects their chemical properties, even if the size difference is small. Therefore, it is important to measure the size and surface structures of AgNPs. In this study, the collision behavior of single AgNP on an electrode is electrochemically monitored while applying oxidizing or reducing potential. In a neutral pH condition, only anodic peak current is observed when AgNPs release Ag^+ ions into the bulk solution. However, in a basic solution, the oxidation of AgNPs produces Ag_xO in the presence of OH^- ions and vise-versa (*i.e.*, reduction of the Ag_xO to reform the AgNPs), resulting in both anodic and cathodic current responses, respectively. We study how the collision of AgNPs depends on their diameters (*i.e.*, 10 nm, 20 nm, and 100 nm) and the type of electrolytes (*i.e.*, KNO_3, $NaNO_3$, KCl) added into a neutral buffer. In addition, nanochannel membranes (*i.e.*, gold electrode coated with polystyrene-*b*-poly(4-vinylpyridine) are used to examine the dependence of pH on the collision behavior of AgNPs. The nanochannels allow only AgNPs smaller than their diameter to reach the electrode and collide with the electrode, achieving size-dependent AgNP detection. At a sufficient negative potential to the hydrophobic nanochannel membrane-coated electrode at pH > pK_a (~4.8), the nanochannels are switched from being dry (*i.e.*, dewetted state) to being wet (*i.e.*, wet state) and the collision of AgNPs is detected on the electrode.

Poster Presentation : **ELEC.P-400**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Ruddlesden-Popper Type Layered Perovskite Oxynitrides for Solar Water Splitting

Yoonji Seo, Jeongsuk Seo*

Department of Chemistry, Chonnam National University, Korea

Solar-driven water splitting for hydrogen energy is sustainable using semiconductors to enhance Solar-to-Hydrogen (STH) energy conversion efficiency. Perovskite-type oxynitrides, AB(O,N)3 (A = La, Ca or Sr; B = Ta, Ti or Nb), have been used as potential semiconductor materials because they are capable of absorbing long wavelengths of visible light, and their band structures straddle the redox potentials of water.[1] Perovskite $CaTa_2N$ absorbs the visible light up to 510 nm wavelengths (Eg = 2.4 eV) and the $LaTiO_2N$ absorbs visible light up to 600 nm wavelengths (Eg = 2.1 eV).[2], [3] However, its valence band maximum (VBM) is very close to the oxidation potential, probably leading to a significant overpotential for water splitting. Herein, we attempted to prepare a new layered perovskite oxynitride $Ca_3Ta_2O_5N_2$ and $La_4Ti_3O_9N_2$ in Ruddlesden-Popper phase with a general formula, A'[An-1BnO3n+1]. The layered perovskite type $Ca_3Ta_2O_5N_2$ was synthesized by nitridation of $Ca_3Ta_2O_8$ prepared through flux-assisted calcination using KCl. In the same way, $La_4Ti_3O_9N_2$ was also synthesized from $La_4Ti_3O_{12}$. The flux method was also used to synthesis the starting oxides at a lower temperature. As a result, the prepared oxynitrides were capable of absorbing visible light. The oxynitride photoanode were fabricated using a particle transfer method followed by the loading of CoOx cocatalyst. More detailed optical properties and water splitting activity of novel layered perovskite oxynitrides will be presented in a poster session.

Poster Presentation : **ELEC.P-401**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Photoelectrochemical Seawater Splitting of Barium-doped Tantalum Nitride in the Wide Range of pH

Seongeon Mun, Jeongsuk Seo*

Department of Chemistry, Chonnam National University, Korea

Tantalum nitride (Ta3N5) has been regarded as a promising semiconductor for photoelectrochemical (PEC) water splitting. The barium doping into Ta3N5 increases the stability of the photoanode for oxygen evolution reaction (OER). [1] The interfacial modification of Ta3N5 photoanode with coating of IrOX caused stable OER in a wide pH range. [2] However, the OER and chlorine evolution reaction (CER) activities of Ta3N5 photoanodes in a wide pH range of seawater electrolytes have never been studied yet. Our group demonstrated OER and CER activities over SrNbO2N photoanode at a neutral pH under AM 1.5G simulated sunlight. [3] The OER or CER activities were found to be dependent on the pH values. Thus, finding a preferential reaction among OER and CER during PEC seawater splitting in a wide pH range is necessary. Herein, we report the competitive OER and CER activities of Ba-doped Ta3N5 photoanode in a wide range of pH. The TaOX layer was sputtered on a Ta foil by radio frequency magnetron sputtering. And coated with Ba(NO3)2 solution as a barium precursor by a dip coating technique. Ba-doped Ta3N5 was synthesized by the nitridation of Ba-coated TaOX. The amounts of gases and ClO- generated on the prepared Ba-doped Ta3N5 photoanode and a Pt counter electrode during seawater splitting at various pH values were quantitatively analysed using gas chromatography and colorimetric detection. Analysing the selectivity of the preferential reaction between OER and CER during PEC seawater splitting in a wide pH range will be presented in a poster session.Reference: ____[1] Nature Communications, 2023, 10 (3), 2566[2] ACS Sustainable Chem. Eng, 2022, 10 (45), 14705-14714[3] ACS Sustainable Chem. Eng, 2023, 11 (5), 1655-1665

Poster Presentation : **ELEC.P-402**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Interface Engineering of BaTaO2N Photoanodes with a Metal Oxide Layer for Efficient Solar Seawater Splitting

Van-Huy Trinh, Jeongsuk Seo*

Department of Chemistry, Chonnam National University, Korea

The perovskite oxynitride BaTaO2N has been considered as a promising photoanode material capable of absorbing visible light up to 660 nm wavelength and appropriate band edge potentials, but exhibited poor photoelectrochemical (PEC) water-splitting activity. [1] The electrocatalyst layers on the surface of BaTaO2N have been demonstrated to be the most efficient way to lower the reaction barrier and promote surface charge injection. [2] In general, the PEC activity of BaTaO2N photoanode is quite high in alkaline solutions but remains modest in neutral-pH electrolytes. However, at the neutral-pH electrolyte, the PEC water-splitting activity of the oxynitride photoanode was impeded by the sluggish kinetics of oxygen evolution reaction (OER).Herein, we report a direct synthesis of nanostructured BaTaO2N thin films on a tantalum substrate through an anodization process and one-step nitridation, which is a promising way to improve the charge transport properties. A metal oxide interlayer was introduced between BaTaO2N and CoOx cocatalyst via radio frequency magnetron sputtering method. Various metal oxide interlayers, such as TiOx, TaOx, MoOx, and AlOx, were applied and their physicochemical properties were also investigated. The introduction of TiOx, AlOx, MoOx interlayer resulted in an enhanced PEC activity in phosphate-buffered 0.5 M NaCl electrolyte at pH 6.5. Further characterization and PEC analyses to clarify the effect of these metal oxide interlayers on the BaTaO2N photoanode activity will be presented in a poster presentation.Reference: [1] Wang, Chizhong, et al. J. Phys. Chem. C 120, 29, (2016) 15758-15764. [2] Higashi Masanobu, et al. J. Am. Chem. Soc. 135, 28 (2013) 10238-10241.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-403**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Mixed metal CoNi-triazole metal-organic framework for an enhanced oxygen evolution electrocatalyst

Natchaya Phongsuk, Sareeya Bureekaew*

School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand

Metal-organic frameworks (MOFs) are emerging as an attractive material for efficient electrocatalytic application. In this study, mixed-metal CoNi-triazole MOF facilely obtained by microwave-assisted methods exhibited electrocatalytic ability for the oxygen evolution reaction (OER). The CoNi-triazole material showed a remarkably low overpotential of c.a. 292 mV at current density of 10 mA cm^{-2} and displayed excellent kinetic properties.

Poster Presentation : **ELEC.P-404**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Improved Electrocatalytic Seawater splitting using Co3O4 Nanocubes with Photodeposited Noble Metal for Selective oxidation

Joon Yong Park, Hyeon Beom Cho[1], Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

[1]*Chemistry, Pusan National University, Korea*

Seawater electrolysis for H2 production is one of the practical applications with a feasible technology. However, the oxygen evolution reaction (OER) with the slow kinetics of the complex multi-electron transfer process at the anode side remains catalytic efficiency deficient and unstable due to their high overpotentials and impurity of nature seawater. Therefore, improving the OER activity and energy conversion efficiency through the design of electrocatalysts is essential. Herein, spinel type cobalt (Ⅱ,Ⅲ) oxide nanocubes (Co3O4NCs) was prepared by hydrothermal reaction, and then carried out with photodeposition of IrO2 and Pd for seawater splitting. To observe their selectivity between oxygen and active chlorine, prepared catalysts with noble metal were exposed to the oxygen evolution reaction (OER) under 0.1 M KOH and chloride oxidation reaction (COR) under 0.5 M and 0.1 M NaCl. The metal photodeposited Co3O4NC showed not only reduced overpotential, but also were preferred for COR than Co3O4NCs. As a result, the onset potential of OER was reduced in the Co3O4NC@IrO2 and the catalytic activity of COR was highly enhanced in the Co3O4NC@Pd, in addition to almost 100% faradic efficiency for COR based on the amount of generated HOCl. In this study, the results of noble-metal-decorated Co3O4NCs suggested the capability of the metal nanoparticles for the improvement of highly selective seawater splitting.

Poster Presentation : **ELEC.P-405**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Advancing Safety and Performance of Fluorine-Free highly concentrated Water-in-Salt Sodium/Calcium-Ion Hybrid Electrolyte for Aqueous Rechargeable Batteries

Thileep Kumar Kumaresan, Myoungho Pyo[1,*]

Department of Advanced Components and Materials Engineering, Sunchon National University, Korea

[1]*Department of Advanced Components and Materials Engineering, Suncheon National University, Korea*

Water-in-salt (WiSE) electrolytes offer a novel approach to expanding the electrochemical window of aqueous electrolytes. Extensively studied TFSI-based WiSEs have demonstrated reliability in energy storage applications. However, the use of perfluorinated anions raises concerns over cost and the environment, particularly in large-scale energy storage. This study explores concentrated electrolytes employing fluorine-free salts, with a focus on nitrate anions as a viable alternative. A new category of inert-cation-assisted WiSE electrolytes (Na/Ca WiSE), comprising sodium nitrate and calcium nitrate, showcases impressive electrochemical performance in aqueous Na/Ca ion hybrid batteries (Na/Ca-HBs). The WiSE electrolyte, concentrated at 25.5 mol kg^{-1} (Na&Ca), exhibits an extensive 2.5 V electrochemical window. This electrolyte mixture offers notable stability, allowing the use of stainless-steel foil as a current collector within aqueous environments. Owing to these unique advantages of the WISE electrolyte, the $Na_4Fe_3PO_4(P_2O_7)$ cathode, and $Ca_{0.14}V_2O_5$ anode can be coupled to construct a prototype of Na/Ca-HBs full-cell using the hybrid electrolyte (Na/Ca WiSE) achieves remarkable performance, competing for the highest reported values for aqueous Na/Ca-HBs. Overall, this fluorine-free cell chemistry offers an environmentally friendly and cost-effective alternative to conventional WiSE systems.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ELEC.P-406**
Electrochemistry
Exhibition Hall C THU 11:00~13:00

Synthesis of F-doped arc graphene and its electrochemical applications

Howoung Shin, Myung Jong Kim*

Department of Chemistry, Gachon University Global Campus, Korea

Modern science and technology rely heavily on the development and application of nanometer-scale materials, and thus the research on carbon-based nanomaterials, graphene and carbon nanotubes, is at the center. These nanomaterials have excellent physical properties and various application possibilities, and innovative applications in various fields such as energy storage devices, electronic devices, and biosensors are expected. To realize these applications, it is essential to manipulate physical properties through the improvement of graft nanostructures along with efficient mass production technology. Furthermore, manipulation through chemical changes to further enhance the properties of nanomaterials is emerging as a very important research topic.In this study, with the goal of improving electrochemical performance, F-doping was performed on graphene using the arc-discharge method. This choice was made primarily for mass production potential and cost effectiveness. In particular, we considered the advantage of relatively low cost compared to other synthesis methods. In addition, F-doping was expected to be doped at the SP3 site, causing changes in the graphene interlayer distance and surface area. This change plays a very important role in electrochemical applications. In particular, the change in the distance between layers is closely related to the charge capacity of an electric double layer capacitor.In the experiment, the structure and property changes of graphene by F-doping were analyzed through TEM, TGA, BET, and Raman analysis. In addition, the effect of F-doping on the electrochemical performance of graphene was evaluated through electrochemical experiments such as CV, EIS, and GCD.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-407**
Electrochemistry
Exhibition Hall C THU 11:00~13:00

Altered Redox Reaction Behavior of Quinone Induced by Nanoconfinement Effects at Microporous Carbon Electrode

Jee Hae Yang, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Nanoconfinement influences molecular interactions and induces alterations in thermodynamic energy, which are not observed in bulk. Here, we have developed a fundamental understanding of the transient redox reaction mechanism of Hydroquinone (H_2Q) and Quinone (Q) within nano-scale pores in an aqueous medium, utilizing cyclic voltammetry (CV) measurements on a microporous carbon electrode. The cyclic voltammogram represents a gradual transformation of the electrochemical redox reaction of H_2Q/Q. This transformation leads to the emergence of stable novel oxidation and reduction reactions within a more negative potential range during successive cycles. Also, Molecular Dynamics (MD) simulations demonstrated the phase separation structures of H_2Q and Q as stable formations in the nanoporous regime. This result demonstrates the unique structures and stabilization of the H_2Q/Q redox reaction under nanoconfinement on a microporous carbon electrode.

Poster Presentation : **ELEC.P-408**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Design and Fabrication of an Adhesive-Based Electrochemical Continuous Flow Reactor with Chemical Resistance

Chanho Song

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

Recent research in the field of chemical synthesis has shown a significant interest in environmentally friendly electrosynthesis. Among these the transition from batch processes to continuous flow processes in electrosynthesis has garnered significant attention due to the numerous advantages it offers. These advantages include reduced electrical resistance, minimized voltage distribution, and a higher surface area-to-volume ratio compared to traditional batch process. These advantages not only facilitate fast chemical conversion while reducing side reactions but also enable an overall higher yield in continuous flow systems. However, designing continuous flow reactors for electrosynthesis has proven challenging due to the requirement for intricate machining process and substantial quantity of expensive electrodes with a large surface area. To address these challenges, a cost-effective continuous flow reactor based on adhesion has been developed. This innovative design utilizes adhesive materials with chemical resistance to connect the anode, cathode, and internal channels. Through this innovative approach, plating solutions flow efficiently along the internal channels and voltage is selectively applied, enabling efficient electroplating. Compared to conventional electroplating methods, this approach offers a practical solution for designing electrochemical continuous flow reactors without the high costs associated with noble metal electrodes and metal molds.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-409**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

The Role of Conducting Polymers Intercalated in Potassium Vanadate Nanofibers for High-Performance Aqueous Zinc-ion Batteries Performance

Yongyeol Park, Seo Young Kang, Young Joon Yoo[1,*], Yuanzhe Piao[2,*], Sang Yoon Park[3,*]

Department of Applied Bioengineering, Seoul National University, Korea
[1]*Advanced Institute of Convergence Technology, Korea*
[2]*Graduate School of Convergence Science and Technol, Seoul National University, Korea*
[3]*Department of Electronic Engineering, Kyonggi University, Korea*

Traditional energy storage system (ESS) relies on lithium-ion batteries (LIBs) due to their high energy density, and low self-discharge. However, since LIBs have cost effects due to raw material supply problems and safety issues due to the use of organic electrolytes, research to replace them is necessary. Aqueous zinc ion batteries (AZIBs) are emerging as suitable candidates for ESS because of safety and eco-friendliness due to the use of aqueous electrolytes, and abundant reserves, low price, high theoretical capacity of zinc metal used as anodes. Nevertheless, vanadium oxide-based materials, which is used as a representative cathode material for AZIBs, has problems such as structural collapse and inherently low electrical conductivity during the intercalation/deintercalation process. To overcome this problem, in this study, PEDOT intercalated potassium vanadate nanofiber (E-PVNF) was synthesized using sonochemistry and used as cathode material for AZIBs. Our developed E-PVNF exhibits remarkable rate capability (124 mAh g^{-1} at 20A g^{-1}) and notable cycle stability (87% retention at 10A g^{-1} after 1,000 cycles). The intercalated PEDOT enhances electrical conductivity while widening interlayer spacing, permitting increased ion storage. Inserted cations and PEDOT function as structural pillars, enhancing stability. The inherent one-dimensional structure shortens diffusion pathways of zinc ions, while structural water within the nanofibers reduces electrostatic interactions, contributing to exceptional rate capability. With safety benefits from water-based electrolytes, impressive electrochemical performance,

and cost-effectiveness, E-PVNF-based AZIBs are expected to open a new horizon as a device that will compose ESS in the future.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ELEC.P-410**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Highly Crystalline Carbon Supports for Fuel Cell Cathodes with Enhanced Catalytic Activity and Stability

Sunguk Noh, Jun Ho Shim[*]

Department of Chemistry, Daegu University, Korea

Research on carbon materials as supports for fuel cell cathodes has been ongoing for several decades. The role of the carbon support is to enhance the dispersion of the catalytic nanoparticles and to facilitate electron transfer between the catalyst nanoparticles and the support. Furthermore, the interaction between the support and metal nanoparticles can alter the electronic structure of the catalyst, which in turn can influence its catalytic activity and stability. Despite the introduction of carbon supports developed through diverse synthesis methods, several unresolved issues remain. These include the corrosion of the carbon support, the penetration and diffusion of catalyst particles limited by specific pore structures, and the reduction of active sites due to strong interactions with the catalyst. In this presentation, we synthesized a precursor of the carbon nitride structures, C_3N_5, and obtained a highly crystalline carbon support through the pyrolysis process. The crystallinity and electrochemical catalytic activity of carbon obtained by introducing various metal catalysts (Mg, Mn, Co) during pyrolysis were comparatively analyzed. A comparative study was also conducted based on the same synthesis method using a C_3N_4 precursor. The carbon support derived from C_3N_5 exhibited superior oxygen reduction reaction (ORR) catalytic activity compared to that from C_3N_4. Notably, due to the highly crystalline carbon structure, it demonstrated enhanced electrode catalyst stability. These results suggest that C_3N_5, produced by a new synthesis method, offers high potential as a catalyst support based on its high crystallinity compared to traditional C_3N_4.

Poster Presentation : **ELEC.P-411**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Efficient and Stable Ammonia Synthesis from MoFe Nanostructures Directly Grown on Carbon Cloth Under Ambient Conditions

Shinyoung Kweon, Jun Ho Shim[1,*]

Daegu University, Korea

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

Molybdenum-iron nanostructured carbon cloths (MoFe/CC) were developed for ammonia synthesis via the nitrogen reduction reaction (NRR) in standard conditions. We measured the catalytic NH_3 yield from NRR in a sealed H-type cell with a Nafion barrier, using electrolyte purged with pure N_2 (or Ar) gas. A variety of analytical methods confirmed the physicochemical attributes and structural aspects of the synthesized catalysts. The combination with a 3:1 molar ratio of Mo to Fe has numerous active sites for interaction with specific molecules, strengthening the bond between active sites and adsorbed N_2. According to previous studies, theoretical calculations indicate that Fe catalysts possess high NRR catalytic activity, while Mo is known for its superior selectivity. The prepared MoFe/CC achieved an NH_3 production rate of 34.32 μg h^{-1} mg^{-1} and a Faradaic efficiency of 57.0% at -0.35 V (vs. reversible hydrogen electrode; RHE). To ensure the NH_3 originated from NRR stimulated by MoFe/CC, we conducted control experiments. For instance, we performed electrolysis on 0.1 M PBS while continuously introducing N_2 at an open circuit potential, observing minimal interference on NRR efficiency from the gas and surrounding environment. Bare CC showed negligible NH_3 production, highlighting the efficacy of our catalyst in ammonia synthesis. We believe this research will guide the design and development of MoFe-based NRR catalysts that are not only more efficient but also possess high stability.

Poster Presentation : **ELEC.P-412**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Enhanced Pseudocapacitor Performance through Mixed Ionic-electronic Behavior of Cationic, Anionic, and Zwitterionic Conjugated Polyelectrolyte Composited with Single-Walled Carbon Nanotubes.

Jinesh Chouhan, Han Young Woo*

Department of Chemistry, Korea University, Korea

Pseudocapacitors (PS) show promise for high-power applications due to rapid charge-discharge kinetics. Conjugated polyelectrolytes (CPEs) are attractive PS electrodes due to their ionic-electronic conductivity. We studied cationic, anionic, and zwitterionic CPEs composited with SWCNTs for enhanced PS performance. Facile chemical synthesis introduced charged functional groups along CPEs' conjugated backbone. Interaction tuning between CPEs and SWCNTs promoted effective charge transfer and surface utilization. Characterization techniques (1H NMR, TEM) elucidated composites' structure and morphology. Electrochemical investigations (CV, GCD) showed improved pseudocapacitive behavior. Charged functional groups facilitated ion diffusion, enhancing capacitance and rate capability. EIS revealed mixed ionic-electronic conduction mechanisms, contributing to superior charge storage and transport. CPE-SWCNT composites demonstrate potential as advanced PS materials, opening new avenues for high-power applications.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ELEC.P-413**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Covalent Conjugation of 'Hydroxide-Philic' Functional Group Achieving 'Hydroxide-Phobic' TEMPO with Superior Stability in All-Organic Aqueous Redox Flow Battery

Jeongmin Yeo, Jinho Chang[*]

Department of Chemistry, Hanyang University, Korea

We show that a covalent conjugation of a 'hydroxide-philic' functional group to TEMPO moiety is the key to effectively mitigating chemical degradation during charging and discharging, which hinders OH–-access to oxoammonium sites in the intramolecular regime, leading to a stable TEMPO-based aqueous organic redox flow battery (AORFB) with long-term cyclability. Thorough quantitative analysis of the degradation of 4-OH-TEMPO in its fully discharged and charged states was performed under various pH conditions; it was confirmed that the strong interaction between the oxidized form (i.e., TEMPO+) and OH– is mainly responsible for the molecular decomposition. Based on this analysis, a TEMPO derivative covalently conjugated with hydroxide-philic functional group was carefully designed and synthesized; in this article, this derivative is designated MIMAcO-TEMPO. The hydroxide-philic MIMAcO functional group intimately attracts OH– before the neighboring TEMPO moiety is exposed to OH–-attack. Once an OH– is combined with the MIMAcO functional group to form the [(OH–→MIMAcO)-TEMPO+] adduct, the oxoammonium site acquires a high electrostatic resistance to OH–. The change in the sequential binding energy of OH– to the MIMAcO functional group and the TEMPO moiety was elucidated by density functional theory (DFT) simulations. The estimated resilient characteristics of the oxoammonium site in MIMAcO-TEMPO+ against OH–, and the resultant structural stability, were confirmed by UV-Vis., NMR, Mass spectroscopy, and electrochemical analyses. In AORFB application, MIMAcO-TEMPO showed a remarkable improvement in capacity decay rate (0.012% per cycle) over 1000 cycles of galvanostatic charge-discharge test, indicating that this is one of the most stable TEMPO derivatives. In addition, based on the highly hydrophilic property of the MIMAcO functional group, a high-concentration

AORFB was successfully demonstrated with 2.5 M MIMAcO-TEMPO, delivering a record-breaking discharge capacity of 57.1 Ah/L.

Poster Presentation : **ELEC.P-414**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

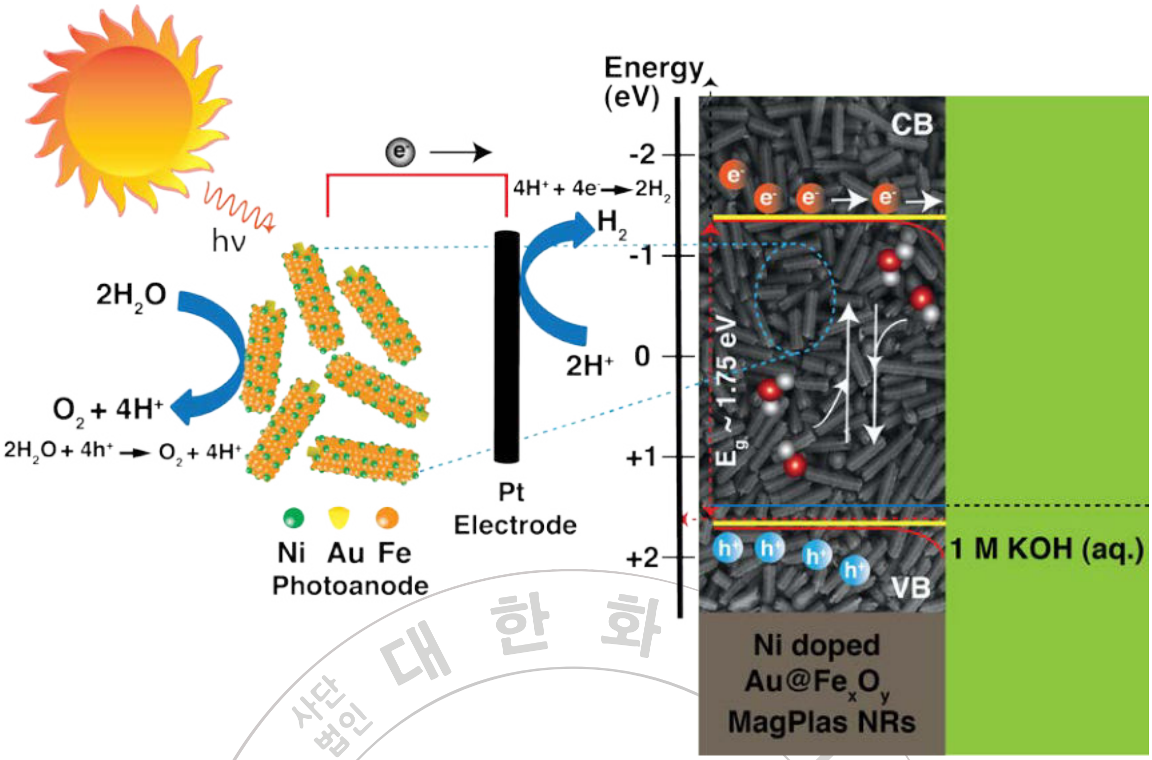
Rugged forest morphology of magnetoplasmonic nanorods for photoelectrochemical water splitting

Goddati Mahendra, Jaebeom Lee[1,*]

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

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

A feasible nanoscale framework of heterogeneous plasmonic materials and proper surface engineering can enhance photoelectrochemical water-splitting performance owing to increased light absorbance, efficient bulk carrier transport, and interfacial charge transfer. This article introduces a new magnetoplasmonic Ni-doped Au@FexOy nanorods based material as a novel photoanode for photoelectrochemical water-splitting. A two-stage procedure produces core-shell Ni/Au@FexOy magnetoplasmonic nanorods. The first step is a one-pot solvothermal synthesis of Au@FexOy. The hollow FexOy nanotubes are a hybrid of Fe2O3 and Fe3O4, and the second step is a sequential hydrothermal treatment for Ni doping. Then, a transverse magnetic field-induced assembly is adopted to decorate Ni/Au@FexOy on FTO glass as an artificially roughened morphologic surface called a rugged forest, allowing more light absorption and active electrochemical sites. Then, to characterize its optical and surface properties, COMSOL Multiphysics simulations are carried out. The core-shell Ni/Au@FexOy magnetoplasmonic nanorods increase photoanode interface charge transfer to 2.73 mA cm−2 at 1.23 V RHE. This improvement is made possible by the rugged morphology of the nanorods, which provide more active sites and oxygen vacancies as the hole transfer medium. The recent finding may lighten plasmonic photocatalytic hybrids and surface morphology for effective photoelectrochemical photoanodes.


hv
e⁻
4H⁺ + 4e⁻ → 2H₂
H₂
2H₂O
O₂ + 4H⁺
2H₂O + 4h⁺ → O₂ + 4H⁺
2H⁺
Pt
Electrode
Ni Au Fe
Photoanode
Energy (eV)
-2
-1
0
+1
+2
CB
e⁻
Eg ~ 1.75 eV
h⁺
VB
1 M KOH (aq.)
Ni doped
Au@FexOy
MagPlas NRs

Poster Presentation : **ELEC.P-415**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Bio-inspired Aqueous Redox Flow Batteries UtilizingDirect Electron Transfer Based BioelectrochemicalInterconversion of NAD H and NAD+

<u>Jeon Yerin</u>, Yoo Seok Lee[1,*]

Korea Polytechnic University, Korea

[1]*Department of Chemical Engineering & Biotechnology, Tech University of Korea, Korea*

As one of renewable energy conversion system, the redox flow battery (RFB) have received great attention as promising energy storage solutions due to their ability to efficiently store and release energy through reversible reduction and oxidation reactions. However, expensive cost of metal redox materials has been issued. In this study, we propose an approach to address this issue by introducing bio-reduction species as a viable alternative to expensive metal redox materials. Diaphorase, an enzyme with intrinsic redox activity and a nanopatterned electrode were combined to create a direct electron transfer (DET) based bioelectrode that can both oxidize NADH and reduce NAD+. An elaborately nano-patterned electrode with a level similar to the size of the enzyme (~10 nm) allows the efficient and stable electric connection between oxidoreductase and electrode. It also eliminates the need for additional redox materials for electron delivery, minimizing thermodynamic and kinetic energy losses. In this work, the immobilization of diaphorase on the complex nanopatterns with high resolution, high aspect ratio, high areal density used for the bioelectrocatalytic oxidation of NADH to NAD+ in electrode. The strategy of DET based inter-conversion of NAD+/NADH at an ultrathin nanotube patterns bioelectrode was harnessed to create a conceptual enzymatic RFB which may be potential candidate for the may be potential candidate for the sustainable energy-storage systems, expanding upon the range of fuels that can be used. The enzymatic RFB’s reliance on bio-redox species showcases its potential to broaden the spectrum of viable energy-storage solutions. This conceptual advancement holds promise as a cost-

effective and sustainable energy-storage solution, propelling the evolution of next-generation energy technologies.

Poster Presentation : **ELEC.P-416**
Electrochemistry
Exhibition Hall C THU 11:00~13:00

Electrochemical biomass upgrading of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid under mild alkaline media.

Eunchong Lee, Yun Jeong Hwang*

Department of Chemistry, Seoul National University, Korea

Biomass has been featured as a fresh carbon source to mitigate the global climate crisis from increased CO_2 concentration and microplastics derived from fossil fuels. 2,5-Furandicarboxylic acid (FDCA) is a product of the oxidation of 5-hydroxymethylfurfural (HMF) obtained from biomass. Furthermore, it holds the promise of substituting a building block in poly(ethylene terephthalate) with poly(ethylene furoate), a more eco-friendly option that also boasts strong mechanical properties. It is well known that electrochemical HMF oxidation (eHMFOR) offers advantages: lower overpotential than oxygen evolution reaction (OER), and production of the value-added product FDCA which is beneficial to oxygen derived from OER. The majority of eHMFOR studies have presented their findings in highly alkaline media (1 M KOH) due to OH- ions as the reactant under the eHMFOR. Nonetheless, applying in a robust alkaline environment becomes undesirable for upscaling with concentrated HMF, as the high OH concentrations render HMF unstable via polymerization to humin. Herein, we designed a reactive Cu-Ni bimetallic catalyst for eHMFOR within a mild alkaline environment achieving the FDCA yield of 97% and faradaic efficiency of 97%. We investigated the Cu-Ni synergetic effect, and distinct tendencies in reaction pathways depending on the various electrolyte conditions. This research would be expected to broaden the range of alkaline, neutral, and acidic pH conditions for eHMFOR in addition to taking the fundamental step to investigate the reactivity to anion effect at the electrical double layer.

Poster Presentation : **ELEC.P-417**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Strategies for enhancing Performance of Nitrogen Reduction Reaction with Cathode Coatings

Yeongbae Jeon, Dongwoo Shin, Yun Jeong Hwang[1,*]

Department of Chemistry, Seoul National University, Korea

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

Ammonia is a primary material in the production of nitrogen-based fertilizers, and it plays an indispensable role in improving crop yields for a growing world population. In addition, ammonia is stable in aqueous state and has a high hydrogen storage capacity per unit volume, making it an attractive hydrogen carrier. Up to the present, industrial production of ammonia relies on the Haber-Bosch method. However, due to the reaction being conducted under high temperatures and pressures, the energy consumption and CO_2 generation are significantly high. Therefore, studies are being conducted on energy-efficient electrochemical ammonia production to replace the Haber-Bosch process. One of them is Nitrogen Reduction Reaction (NRR), which is a synthesis of ammonia by electrochemically reducing a nitrogen. Non-aqueous Li-mediated NRR with tetrahydrofuran as solvent has advantages of low error due to nitrogen impurities (e.g. NO_x) and high ammonia yield. In this study, the Faradaic efficiency of Li-mediated NRR was increased by electrodeposition and catalyst spray coating on the surface of the electrode. Through ammonia quantification using UV-vis spectroscopy, it was confirmed that NRR efficiency increased when bismuth or copper was used. From this study, the results suggest that the catalytic effect can improve NRR performance by coating the cathode with catalysts.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ELEC.P-418**
Electrochemistry
Exhibition Hall C THU 11:00~13:00

Effect of metal oxides on product selectivity and current density of the Cu-based catalyst during electrochemical CO2 reduction

Dayeon Kim, Yun Jeong Hwang[1,*]

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

Copper is almost the only metal that can produce a wide variety of multi-carbon products such as ethanol, ethylene, and acetate through electrochemical CO2 reduction. To produce the demanded amount of C2+ products with Cu-based catalyst, various factors such as grain boundary, subsurface oxygen, surface charge state, and facet can be modified. These factors can be controlled by introduction of polymers, morphology or size control through synthesis. In this study, we investigated whether the introduction of metal oxide into Cu as a co-catalyst material leads to performance changes in product selectivity and current density. Also, to produce relatively large amounts of products, it is necessary to use a membrane electrode assembly (MEA), which can achieve high current density by implementing a zero-gap system. However, in the MEA, CO2 injected from the cathode side can react with OH- that crosses the membrane during the reaction to produce carbonates. This crossover leads to a loss of CO2 that should be used as a reactant, resulting in poor performance. Therefore, we also studied how the introduction of metal oxides changes the performance of catalysts in the MEA.

Poster Presentation : **ELEC.P-419**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

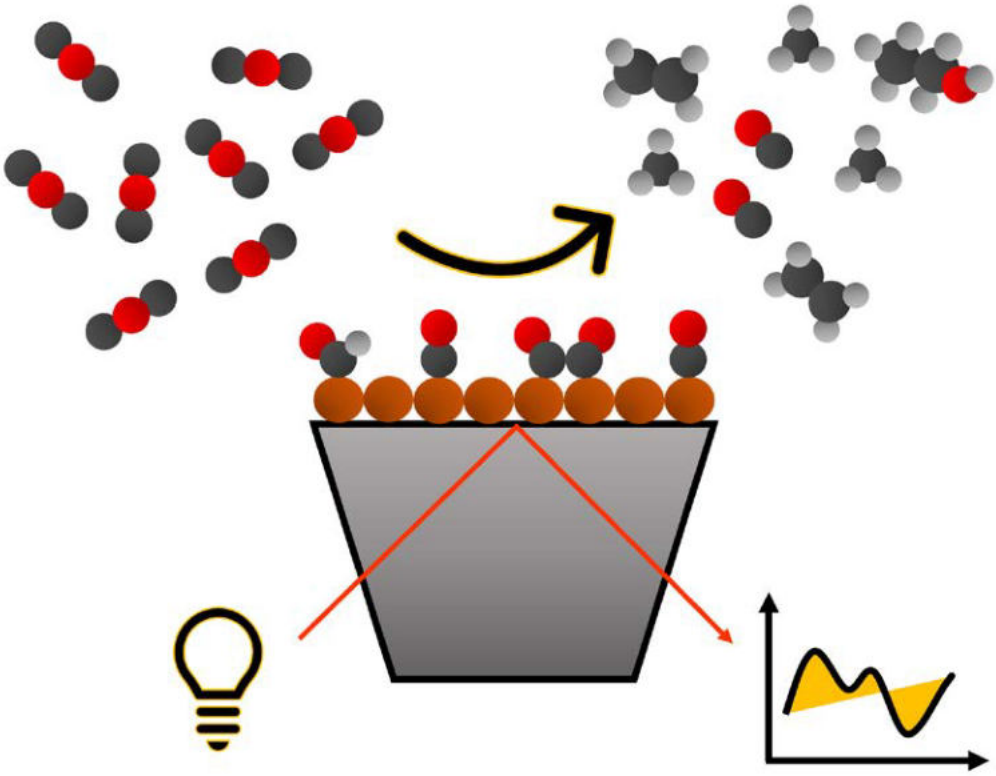
Elucidating the Electric Field Effect Controlled by Cation Concentration on the Cu in the Acidic CO2RR

Suhwan Yoo, Yun Jeong Hwang[1,*]

Department of Chemistry, Seoul National University, Korea

[1]Chemistry Department, Seoul National University, Korea

As climate change emerges, the importance of decarbonization is being stressed day by day. One strategy that has received the most attention is the electrochemical conversion of carbon dioxide. Recently, acidic media is getting attention to reach the industrial level. Due to the rich hydronium ion in the acidic media, HER is favored compared to the CO2RR. Introducing the cation can solve the problem by inhibiting the hydronium ion migration and stabilizing the intermediates of the CO2RR. However, despite the importance of the cation, deep investigation of the cation effect in acidic media is not proceeded so far. So, in here, we introduced in situ ATR-SEIRAS (Attenuated Total Reflection–Surface Enhanced Infrared Spectroscopy) which can detect the adsorbate and interfacial species to examine the interface in the acidic condition. Copper (Cu) is the only metal which can synthesize the C2+ product due to the optimal binding strength. Cu catalyst can generate adsorbed CO (*CO), key intermediate for C-C coupling, which means that it is suitable for measuring the electric field with the stark tuning rate (STR). We confirmed electric field strength can change by increasing the cation concentration, and the *CO species are observed only plateau potential range, hydronium ion depletion region near the catalyst. We found the cation can accumulate effectively at the plateau potential range in the high cation concentration. While, at the low cation concentration, the cation cannot accumulate stably, and so HER can occur easily. The high selectivity toward to the CO2RR over the HER in the high cation concentration can be originated from the stably formed cation layer.



Poster Presentation : **ELEC.P-420**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Influence of Sulfur Doping Concentrations on the Electrochemical Performance of Hollow NiFe-LDH in Oxygen Evolution Reactions

Sojin Jung, Jun Ho Shim[*]

Department of Chemistry, Daegu University, Korea

Developing cost-effective electrocatalysts with optimal oxygen evolution reaction (OER) kinetics is crucial for applications in water splitting, carbon dioxide reduction, and metal-air batteries, but this remains a significant challenge. The complexity and slow kinetics of the multielectron transfer process highlight the need for highly efficient electrocatalysts. In this presentation, we discuss the synthesis of sulfur-doped hollow NiFe layered double hydroxide (NiFe-LDH) and investigate its efficacy as a catalyst for the OER. The weight ratio of thioacetamide to NiFe-LDH was adjusted and synthesized at 0:10, 4:6, 6:4 and 8:2. Notably, the S-doped NiFe-LDH optimized at a 6:4 weight ratio of thioacetamide to NiFe-LDH exhibited outstanding OER catalytic performance, requiring only an overpotential of 235 mV to achieve a current density of 10 mA cm^{-2}, outperforming other reference catalysts. For comparison, we also synthesized transition-metal-substituted nanocomposites, including CoFe, NiMn, and CoMn, using optimal weight ratios of thioacetamide to NiFe-LDH. The introduction of sulfur not only serves as an effective strategy for creating superior OER electrocatalysts but also offers a new perspective on understanding electrocatalysts at both electronic and atomic levels.

Poster Presentation : **ELEC.P-421**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Correlations between the Impedance and Compressive Strength of Hardened Cement According to the Aggregate Type

Jinju Kim, Hyun Ju Yang, 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, which represents the boundary between the aggregate and paste inside concrete, have primarily relied on destructive tests, with non-destructive tests attracting only little attention until recently. This study assessed the interfaces of concrete with lightweight aggregates based on electrochemical impedance spectroscopy (EIS) for high-strength concrete and examined the possibility of estimating the compressive strength of concrete through non-destructive testing using EIS. The experimental results revealed that the impedance of hardened cement increased with increasing compressive strength and aggregate density. In particular, when the impedance measurement results were represented as a Nyquist plot, the value of Rb, 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 obtained Nyquist plot and better understand the correlation between cement aggregates and impedance. Consequently, the compressive strength was found to increase with the value of R1 in the equivalent circuit. Therefore, this study developed a new method for determining the compressive strength of hardened cement using a non-destructive experimental method.

Poster Presentation : **ELEC.P-422**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Effect of Additives on Electrochemical Nitrogen Reduction Reactions in Non-aqueous Lithium-mediated Systems

Dongwoo Shin, Yeongbae Jeon, Yewon Hong, Yun Jeong Hwang[*]

Department of Chemistry, Seoul National University, Korea

Ammonia (NH3) plays a pivotal role as a crucial component in fertilizers and exhibits promise for facilitating the safe storage and transportation of hydrogen energy, thereby potentially supplanting fossil fuels. However, prevalent industrial methods for NH3 production entail high-temperature, high-pressure procedures that yield substantial CO2 emissions, contributing to environmental degradation. Non-aqueous Li-mediated nitrogen reduction reaction (NRR) is a novel avenue of research that has the advantages of high current density along with suppression of competitive reactions such as hydrogen evolution reaction and high mass transfer of nitrogen molecules, resulting in significant NRR efficiency. In a non-aqueous system, the reduction of Li ions, the reaction between Li and N2 gas, and the reaction between H ions and electrons to produce NH3 proceed in one cycle. This investigation centered on refining the solid electrolyte interface (SEI) through the incorporation of minor additive quantities, yielding remarkable enhancements in NRR yield and Faradaic efficiency. The optimization of interfacial dynamics necessitates the manipulation of various parameters, encompassing the solvent, the material of the reaction electrode, the type and concentration of salts, and the hydrogen shuttle material. Complementary techniques such as electron microscopy and X-ray analyses were employed to scrutinize the morphology of the SEIs, crystal structures, and material states. Isotope testing, experiments under argon conditions, and multiple reproducible experiments confirmed the stability of the system. The prospect of enhancing NRR efficiency through additives is expected to be a pioneering step in showing the importance of SEI in NRR and the direction of future research.

Poster Presentation : **ELEC.P-423**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Improving the Electrochemical Oxygen Evolution Activity of Conventional Nickel-Iron Catalyst through Anion Regulation

Yewon Hong, Juhyung Choi[*], Yun Jeong Hwang[1,*]

Department of Chemistry, Seoul National University, Korea

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

Electrochemical water splitting, composed of Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER), has been received attention because it generates clean hydrogen energy with only water as a byproduct. Meanwhile, producing sufficient amount of hydrogen gas and meeting industrial requirements still remain a challenge due to the OER, which consumes more energy and thus limits the overall reaction rate. IrO2 and RuO2 has been acknowledged as highly active state-of-the-art catalysts, but its low stability, scarcity, and high market price makes its industrial usage impossible. [1] Therefore, a means to replace it with abundant transition metal-based materials is still in demand.Among the various compositions of transition metal-based catalysts, NiFe based electrocatalysts were found to be particularly active and have the capability to replace the precious metal catalysts. [2] However, after long periods of uptime, Fe segregation of the catalyst was inevitable, creating a phase segregation which resulted in a loss of catalytic activity. [3] Here we regulated the anion of the NiFe catalyst by introducing boron through a simple and facile method, and thus were able to significantly lower the overpotential and increase the overall stability. The results of this study provide and emphasize the importance of anion regulation as an effective method to enhance transition metal-based OER catalysts, contributing to the industrialization of hydrogen.References[1] W. H. Lee et al. Electroactivation-induced IrNi nanoparticles under different pH conditions for neutral water oxidation. Nanoscale, 2020, 12, 14903[2] M. Moloudi et al, Layered Double Hydroxide Templated Synthesis of Amorphous NiCoFeB as a Multifunctional Electrocatalyst for Overall Water Splitting and Rechargeable Zinc–Air Batteries, Advanced Energy

Materials, 2023, 13, 2203002[3] C. Kuai et al, Phase segregation reversibility in mixed-metal hydroxide water oxidation catalysts, Nature Catalysis, 2020, 3, 743-753

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ELEC.P-424**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Spontaneous Zn-CO2 Battery for Efficient CO2 Electroreduction

DongYoon Lee, Yongsung Jo, Dongil Lee[1,*]

chemistry, Yonsei University, Korea

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

Electrochemical carbon dioxide reduction reaction (CO2RR) to value-added products is a promising strategy to reduce atmospheric CO2. However, conventional CO2RR systems typically rely on external electric energy derived from fossil fuel combustion, which limits their sustainability benefits. In contrast Zn-CO2 battery is an emerging kind of energy device, which has fast kinetics for Zn oxidation and spontaneously converts CO2 into value-added chemicals through CO2RR process. In this poster, we present a novel aqueous Zn-CO2 battery incorporating a gas diffusion electrode and a thin layer electrolyzer that enables highly efficient Zn-CO2 battery performance with direct supply of CO2 and minimal ohmic drop. The thin layer Zn-CO2 battery employing gold nanocluster catalyst exhibited a remarkable current density and power density (200 mA cm–2 and 21 mW cm–2, respectively) with exclusive CO production. Even in diluted CO2 gas (0.2 atm of CO2), Zn-CO2 battery generated current density of up to 100 mA cm–2 with CO selectivity exceeding 90% and high durability was confirmed over 24 hours at 100 mA cm–2 with mechanical recharge. Furthermore, anode recovery system was developed, in which Zn was recovered as ZnO

Poster Presentation : **ELEC.P-425**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

Dopant Effects on the Electrochemical Hydrogen Evolution Reaction Catalyzed by Heterometal Doped Silver Nanoclusters

Jiyeon Shin, Hanseok Yi[1], Dongil Lee[1,*]

chemistry, Yonsei University, Korea

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

A superatom is a cluster of atoms behaving in certain ways like an element. Ligand-protected metal nanoclusters (NCs) are also considered as superatomic materials. Due to their atomically precise structure identification, the NCs have potential to be used as an ideal platform for understanding structure-property relationships. In NC systems, heterometal doping is a promising strategy for fine tuning the physicochemical properties of the parent NCs. In this presentation, we report synthesis and electrocatalytic applications of $Ag_{25}(SR)_{18}$ (SR = thiolate) NCs doped with heterometals (Au, Pd, Pt, RhH, IrH). Combined experimental and theoretical studies revealed that the RhH and IrH dopants were superatomic constructs of Pd and Pt atoms, respectively. To verify the dopant effects on their electrocatalytic hydrogen evolution reaction (HER) activity, we conducted acid and alkaline HER catalyzed by heterometal doped Ag NCs. Under acidic conditions, all doped Ag NCs exhibited comparable HER activities regardless of the dopants. In contrast, the doping effect of the catalyst NCs was evident in alkaline HER. Further kinetic isotope effect experiments and theoretical studies were conducted to reveal the origin of the dopant effects. Interestingly, among the doped NCs $RhH@Ag_{24}(SR)_{18}$ showed the highest alkaline HER activity, which is even higher than that of the Pt-doped NC. Moreover, $RhH@Ag_{24}(SR)_{18}$ exhibited stable HER activity during the 24-hour constant potential electrolysis.

Poster Presentation : **ELEC.P-426**

Electrochemistry

Exhibition Hall C THU 11:00~13:00

[Withdrawal] The Crumpled Interlayered Architecture of Copper Tungsten Sulfide decorated reduced Graphene Oxide Nanocomposite as Advanced air cathode for Flexible Zinc–Air Battery

Bee Lyong Yang

Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **EDU.P-444**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

Textbook analysis and science teachers' awareness of the conditions under which phase diagram is drawn

YoungHa Hwang, **Seounghey Paik**[1,*]

Korea National University of Education, Korea

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

In this study, in relation to the phase diagram of the 2015 revised curriculum Chemistry II textbook, the textbook descriptions related to the conditions under which the phase diagram is drawn were analyzed and teachers' perceptions were investigated. As a result of the study, even though the phase diagram is a graph made by assuming a closed system, all textbooks do not directly mention the term closed system, and only two of the six textbooks used for analysis solve the concept of a closed system and indirectly was describing. In this regard, when seven incumbent teachers were selected as study subjects and presented with the task of interpreting the situation in an open system as a phase diagram, only one teacher mentioned the difference between open and closed systems. This can be interpreted as the fact that even teachers who teach students in the field formed a misconception because the textbook did not specify the conditions for drawing a phase diagram. Even in the case of textbooks that indirectly solved closed systems, it was clearly revealed that the movement of matter was prohibited, but it was confirmed that there was no description of whether energy could be moved. It was confirmed that the problem that was difficult for the professor was drawn as a process. In order to solve this problem, it is necessary to specify in the curriculum achievement standards and textbooks that the phase diagram is true in a one-component closed system.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-445**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

The effect of What-If Activities on Student Discourse in Inquiry-Based Investigative Science Education(ABI)

Seongdae Park, Jeonghee Nam[1,*], Jihun Park[1], Hyeongtak Yun[1]

Chemistry education, Pusan National University, Korea

[1]*Department of Chemical Education, Pusan National University, Korea*

This study aimed to investigate the impact of What-If activities on the refutation and characteristics of discussion processes among high school science students in an Argument-Based Inquiry(ABI) science class with the addition of What-If activities. To achieve this, four classes of first-year high school students (a total of 70 students) from a science high school located in a metropolitan city were selected as participants. Two classes (35 students) were assigned to the experimental group, where the Argument-Based Inquiry science class with What-If activities was conducted, while the other two classes (35 students) were assigned to the control group, where a regular Argument-Based Inquiry science class was conducted. Starting from August 2023 and continuing for one semester, the experimental group participated in the Argument-Based Inquiry science class with What-If activities for four different topics, while the control group participated in a regular Argument-Based Inquiry science class. To understand the changes in the types and frequencies of refutations, the classroom discussions in the ABI class of the experimental group were compared with the What-If discussions within the same class. Additionally, to explore the changes in the characteristics of the discussion processes, the classroom discussions in the ABI class of the experimental group were compared with the classroom discussions in the ABI class of the control group. Based on these results, strategies will be proposed to encourage students to engage in high-level discussions that incorporate refutations.

Poster Presentation : **EDU.P-446**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

Direction of Pre-service Chemistry Teacher Education for Change in Cognition of the Nature of Model

Najin Jeong, Seounghey Paik*

Department of Chemical Education, Korea National University of Education, Korea

In science, models are an important means and tool to connect natural phenomena and theories. Through models, complex natural phenomena can be explained and predicted by simplifying and abstracting them, and scientific facts can be communicated. Models have been consistently emphasized in science education in Korea. In particular, the 2022 revised curriculum emphasizes the importance of developing and utilizing models and calls for a more active approach to models as the school level or grade level increases. In order to properly develop and use models in science classes, the teachers' understanding of the model is necessary, and understanding the model must be preceded by cognition of the nature of model. However, in a study investigating teachers' cognition of the nature of model, models were perceived as representing reality or only as a representational tool for visualizing concepts. Research was also conducted on training programs to improve teachers' cognition, but it was difficult to bring about a change in the epistemological understanding that models are a core element of science and a tool for constructing knowledge. Cognition of the nature of model can be seen as closer to belief than simple scientific knowledge, and it is difficult to change once the cognition is formed. Therefore, it is necessary to achieve a correct cognition of the nature of model through systematic education from the stage of pre-service teacher education. In this study, a pre-service teacher education program consisting of four stages was developed and applied: 'Observation of natural phenomena', 'Design of model', 'Implementation of model through technology', and 'Evaluation and modification of model'. Based on the results, we would like to propose a direction for pre-service chemistry teacher education to change cognition of the nature of model.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **EDU.P-447**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

The Effect of Advanced Science Technology-Based Education Programs on Science Career Orientation and Attitude Toward Chemistry

Jiyun Yang, Hyunjung Kim[1,*], Hyuck Jin Lee[1], Sungyool Bong[1]

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

This study investigated the effects of the science education programs based on the advanced science technology on students' science career orientation and their attitudes toward chemistry. The participants were experienced two types of science education programs held in September and October 2023, developed at the Starbridge Chungcheong Center in teacher participation research project. The effectiveness of the program was assessed by t-test with a one-group pre-posttest design. The survey instruments for measuring science career orientation and attitude toward chemistry consisted of 20 items each on a five-point Likert scale. The pre- and post-surveys were conducted online. In this study, we analyzed science career orientation and attitude toward chemistry as follows. Science career orientation is categorized into preference for science learning, preference for science career, awareness of science career value, and need for science career information. For attitude toward chemistry, it was categorized under four categories: interest and utility, anxiety, intellectual accessibility, fear, and emotional satisfaction. Through this analysis, the purpose of this study is to prove the educational value of a program that applies advanced science technology to chemistry education and to provide insight into its implications.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-448**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

A Modular Robotic Platform for Chemical & Biological Research

Sung-Ho Lee, Jiae Park[1], Albertus Ivan Brilian[1], Kwanwoo Shin[2,*]

Institute of Biological Interface, Sogang University, Korea
[1]*Chemistry, Sogang University, Korea*
[2]*Department of Chemistry, Sogang University, Korea*

In recent years, robotic arms have become a common tool to replace human operators in various environments and are expected to play an important role in automating laboratory tasks. Nevertheless, chemical or biological experiments are still considered to be areas that cannot be easily replaced by robots, as the success of the experiment depends on human factors such as the researcher's skill and experience. In this work, we introduce the concept of utilizing robots for automation and remote control of tasks specific to chemical and biological experiments, as well as general tasks performed by researchers. We present the development of a 'chem-bot', a modularized robotic platform consisting of a robotic arm, auxiliary devices, and software. The platform enables fully automated or remote control of liquid dispensing, mixing, and various chemical reactions, and key experiments in biology such as cell seeding, culture, and genetic manipulation. It can be remotely operated in real time through its own online program. This modular robotic platform represents a breakthrough in laboratory automation and promises efficiency, reproducibility, and scientific advancement over human-performed experiments.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-449**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

How Hydrogen Energy and Artificial Intelligence (AI) will be Educating at the Chemistry Classroom?

Raeyoung Lee, Sangwoo Bae[1], Park Geon Hee[2], Hyuck Jin Lee[3], Hyunjung Kim[3], Sungyool Bong[3,*]

Kongju National University High School, Korea
[1]*Daejeon gao high school, Korea*
[2]*Kongju National University, Korea*
[3]*Department of Chemistry Education, Kongju National University, Korea*

Hydrogen energy is becoming increasingly important as a clean and sustainable source of energy. Understanding its chemical properties and reaction mechanisms is fundamental in the field of chemistry education. By gaining knowledge on hydrogen, one can actively contribute to the development of new technologies and materials for future green energy innovation. Here are reasons why hydrogen energy should be taught in chemistry education: 1. Clean and Sustainable Energy: Hydrogen energy is considered a clean source of energy as its combustion only produces water vapor as a byproduct. Introducing students to this renewable and sustainable alternative can encourage them to think about ways to reduce our dependency on fossil fuels, potentially minimizing our impact on the environment. 2. Addressing Climate Change: By learning about hydrogen energy, students can form a better understanding of climate change and how it is linked to our energy consumption. Educating them on the benefits and potentials of hydrogen energy can inspire them to become future leaders and innovators in renewable energy technology. 3. Advancements in Technology: The field of hydrogen energy offers exciting opportunities for research and technological advancements. Teaching about hydrogen energy in chemistry education can inspire students to explore various aspects of fuel cells, hydrogen storage, and conversion technologies. This, in turn, can lead to breakthroughs in energy storage and transportation systems. In this research, we propose the chemistry education model for basic concept and application of hydrogen energy with entry program and experimental based on Korea Education Curriculum.

Poster Presentation : **EDU.P-450**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

The Perceptions of Chemistry Teachers regarding Science Experiment Safety and Chemicals

Hyein Park, Hyunjung Kim[1,*], Jiyun Yang[2]

Kongju National University, Korea

[1]*Department of Chemistry Education, Kongju National University, Korea*

[2]*Chemical Education, Kongju National University, Korea*

Due to the recent increase in safety accidents in science laboratories and strengthened legal regulations related to chemicals, science experiments in Korean schools are on the decline. Accordingly, the Ministry of Education has established a support system to set up a safe science laboratory and is promoting an increase in science experiments based on this. In this context, this study aimed to investigate science teachers' perceptions of science experiment safety and chemical management. It particularly targets teachers in charge of chemistry subjects, who are known to conduct the most hands-on activities involving chemicals. The participants included 103 chemistry teachers, with 35 from middle schools and 68 from high schools. The questionnaire, adapted and translated for the Korean context based on previous studies about chemical management and anxiety, consists of a total of 45 items, divided into four sections: 12 on laboratory safety equipment, 8 on chemical storage and management, 13 on laboratory safety guidelines and education, and 12 on experiment anxiety and experiment activation. The sections on lab equipment, storage, and guidelines used a 3-point Likert scale, while anxiety and activation used a 5-point Likert scale with open-ended questions. The response data for frequencies and averages were analyzed using SPSS 27.0, comparing perceptions by school level, gender, and experience. The results of this study examined the status of chemistry teachers' perceptions regarding laboratory safety equipment, chemical storage and management, laboratory safety guidelines and safety education, and laboratory anxiety and science experiment activation. Significant differences based on gender were observed, particularly in the context of science experiment anxiety.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-451**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

A Comparison of Chemistry Textbooks in Elementary and Middle Schools in Mongolia and Korea

Gantumur Darisuren, Hyun Kyung Kim[1,*]

Jeonbuk National University, Korea

[1]*Chemistry Education, Jeonbuk National University, Korea*

The purpose of this study is to compare elementary and secondary chemistry textbooks in Mongolia and Korea, and to prepare basic data to be used when revising chemistry textbooks in both countries in the future. In order to conduct this study, the contents of the chemistry curriculum of the textbooks prepared according to the curriculum in Mongolia and Korea were analyzed. After that, the overall composition of the chemistry field and the teaching and learning method were compared and analyzed. In order to compare and analyze the overall composition of the textbook and the teaching and learning method, the analysis framework was developed by reorganizing the contents presented in the existing comparative study. As a result of comparing textbooks from both countries with the developed analysis framework, there was a difference in the number of large numbers, pages, illustrations, and problems of elementary and secondary chemistry textbooks. In addition, Mongolian textbooks focus more on strengthening students' knowledge through descriptive examples and descriptive questions in each class, and Korean textbooks focus on meta-cognition and creativity development, including creativity and self-evaluation questions at the end of each class. The implications for the comparative analysis results are as follows. Mongolia needs to review the appropriateness of the revision of textbooks because the number of illustrations, which are visual materials to arouse students' interest, and Korea needs to reduce the amount of illustrations because high schools need to solve practice problems or tasks rather than visual materials. In addition, there is no evaluation of the small unit that is completed after the small unit is finished in Mongolian textbooks. Based on these points, efforts to improve textbooks in both countries are needed in the future.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-452**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

A Study on Science Educators' Perceptions of the Nature of Science Through the Reconceptualized Family Resemblance Approach

Seong Hye Kim[*], **Seounghey Paik**[*]

Department of Chemical Education, Korea National University of Education, Korea

In this study, we aimed to explore the perceptions of science major teachers based on a reconceptualized family resemblance approach to the nature of science. Twelve graduate students who were serving as science teachers participated in the research. They responded to survey questions from Kaya et al. (2019)'s RFN questionnaire (6 categories, 70 items) and provided explanations for their responses. Additionally, we compared the characteristics of Korean science teachers with the results of previous studies that investigated the nature of science using the same questionnaire.Comparing the results of RFN surveys conducted on UAE science teachers and prospective teachers with those of Korean science teachers, differences were observed in various domains. In the aims and value area, 4 out of 7 items showed differences. In the scientific practices area, 4 out of 13 items differed. In the scientific method area, 5 out of 9 items differed. In the scientific knowledge area, 4 out of 9 items differed. In the social-institutional aspect, 7 out of 16 items differed, and in the educational applications area, 6 out of 16 items differed.During the process of analyzing the survey results of Korean science teachers along with interview content, it was challenging to maintain consistency in the interpretation of teacher perceptions, even for the same responses, due to differences in criteria for Likert scales and interpretations of survey questions among research subjects. Therefore, in this study, we reclassified the Likert 5-point scale into 'Consent,' 'Partially Consent,' 'Dissent,' and 'I don't know' and conducted the analysis. When analyzed with different scales, more than 50% of the items showed clearer insights into perceptions, and it appeared to reduce confusion in teacher choices.Overall, teachers generally had a consensus on RFN, especially in the social-institutional domain, where they mostly agreed. However, some items, particularly in the aims and value domain, had a high percentage of 'I don't know' responses, and there

were also disagreements in the scientific method and knowledge domains. Detailed insights into the perceptions of science major teachers about the nature of science can contribute to their NOS education, and we intend to propose improvements for the RFN questionnaire items.

Poster Presentation : **EDU.P-453**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

Analysis of Online Overseas Educational Voluntary Activities with Cultural-Historical Activity Theory

DaYeong Jang, Jeongho Cha*

Department of Chemistry Education, Daegu University, Korea

Educational voluntary activity is recognized as a significant contributor to the pursuit of the Sustainable Development Goals (SDGs), a set of 17 global objectives aimed at ensuring quality education and fostering lifelong learning. This type of activity is not only prevalent domestically but also holds international prominence. However, the emergence of the COVID-19 pandemic necessitated a transformation in the realm of overseas educational voluntary endeavors, prompting a shift towards online formats. In this study, we employ the Cultural-Historical Activity Theory (CHAT) to examine a two-year span of online overseas educational voluntary activities and compare the results with those of their traditional face-to-face counterparts based on the literature. We particularly delve into the tools employed, such as Zoom, and the role distribution, including co-teachers, within the framework of the six key components: subject, object, tools, community, rules, and role distribution. The primary goal is to present a detailed understanding of the advantages and limitations inherent in online overseas educational voluntary activities. Through this analysis, we aim to provide invaluable insights that can facilitate the enhancement of the effectiveness of online activities.

Poster Presentation : **EDU.P-454**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

An Analysis of Pre-service Science Teachers' Lessons in Teaching Practice from the Sociocultural Perspective Using CHAT

Minhwan Kim, Sunghoon Kim[1], Taehee Noh[2,*]

Center for Educational Research, Seoul National University, Korea

[1]*Seoul National University, Korea*

[2]*Department of Chemistry Education, Seoul National University, Korea*

In this study, we analyzed the process of pre-service science teachers' designing and implementation of lessons in teaching practice from the perspective of CHAT. Five pre-service teachers attending the Department of Chemistry Education at the College of Education in Seoul participated in this study. We observed their teaching practice, collected documentary data, and conducted in-depth interviews. The data were analyzed using the constant comparative method based on grounded theory. The analyses of the results reveal that, due to the lack of authority to make decisions for lesson design, pre-service teachers faced difficulties and had direct conflict with teachers. In addition, it was difficult for them to obtain sufficient contextual information for lesson design even through subject orientation and classroom observation, which made it difficult for them to design lessons. When consecutive lessons were taken by several pre-service teachers, there were many problems such as poor continuity of lessons. Given limited authority to assess students, they conducted additional assessments. They showed a lack of professionalism when conducting assessments. The cause of this could be found in the curriculum of the College of Education. Some ways to provide better teaching practice based on the results are discussed.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **EDU.P-455**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

An Analysis of Discourse in Middle School Students' Small Group Learning with Augmented Reality

Nayoon Song, **Taehee Noh***

Department of Chemistry Education, Seoul National University, Korea

This study analyzed discourse in middle school students' small group learning using augmented reality. Eight 8th grade students took classes using augmented reality in solubility, boiling and melting points. These classes were carried out twice and all the classes were videotaped and recorded. Every students participated in a semi-structured interview. In the types of knowledge building discourse, the proportion of knowledge sharing and knowledge construction was similar. Beneath the knowledge sharing, the proportion of introductory level discussion was higher than identifying key elements of augmented reality. Recalling existing knowledge rarely appeared. Under the knowledge construction, the proportion of advanced level discussion was the highest and the proportion of sharing and critiquing ideas at different level and efforts to rise above current levels of explanation was similar. The introductory level discussion and identifying key elements of augmented reality were developed into efforts to rise above current levels of explanation and sharing and critiquing ideas at different level. Visualized results of knowledge building processes showed all the students' graph drew an upward curve though cumulative number of impact value was different by each students. As a result of the study, effective ways of improving small group learning using augmented reality are discussed.

Poster Presentation : **EDU.P-456**

Chemistry Education

Exhibition Hall C FRI 11:00~13:00

A Comparative Analysis Study of South and North Korea Chemistry Textbook on Acid·Base and Oxidation·Reduction Concept

Wonjun Hwang, Heesook Yoon*

Department of Science Education, Kangwon National University, Korea

The purpose of this study is to compare the textbooks from 2015 revised curriculum of South Korea and North Korea's Kim Jong-un era on the concepts related to 'acid and base' and 'oxidation and reduction'. To achieve this, we compared when to learn, what to learn, and procedures, experiments, etc.. As a result of the study, the concept related to acid and base had the following characteristics. First, spiral education is provided for a long period of time from the 5th to 6th grades of elementary school to the 3rd grade of high school in South Korea, but North Korea only learns acid bases for 2 years from the 3rd grade of elementary middle school to the 1st grade of high middle school. Second, in South Korea, the concept of acid and base is learned in the same unit at the same time, whereas in North Korea, acid and base are learned in different units. Third, in North Korea, there is little content related to the neutralization reaction, and it mainly deals with the production of salts and their salts due to the neutralization reaction. Concepts such as neutralization fever, quantitative relations, and neutralization appropriateness covered in South Korean textbooks were not included. Fourth, the two Koreas have similar experiments related to the properties of acids and bases, but North Korean textbooks have only one experiment related to neutralization reactions, which is very small compared to South Korean textbooks. In other words, in the case of North Korea, salt caused by the neutralization reaction was emphasized rather than the neutralization reaction itself, and in the case of South Korea, various characteristics of the neutralization reaction were closely studied. The concept related to 'oxidation and reduction' had the following characteristics. First, North Korea was introducing oxidation water before learning the concept of redox. Second, North Korea was learning redox spirally from elementary middle school grade 2 to high middle

school, so it was learning earlier than South Korea, which deals with redox of organic compounds, and explosives.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **EDU.P-457**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

Development and Educational Application of Bisphenol A Detection Experiments

<u>Seung Bin Choi</u>, Heesook Yoon*

Department of Science Education, Kangwon National University, Korea

Bisphenol A (referred to as BPA) is an environmental hormone that is widely used, such as receipts, baby bottles, and food cans, but has a similar effect to estrogen. Recently, as risks have become widely known, BPA regulations have been made and consumers are relieved by the phrase "BPA free," but there is still a risk of similar alternatives. The purpose of this study is to develop and apply educational programs to change students' understanding and perception of environmental hormones. To this end, a BPA detection experiment in receipts was devised and an environmental hormone-related education program that can be used in secondary school was developed.

Poster Presentation : **EDU.P-458**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

Comparison and Analysis of Conceptual Levels and Misconceptions of Korean and American Students Using AAAS Conceptual Testing Tools for Atomic, Molecular, and Matter Conditions

Heesook Yoon, **Heesook Yoon***

Department of Science Education, Kangwon National University, Korea

The purpose of this study is to compare and analyze the level of concept of the state of atoms, molecules, and substances of Korean and American students. As a test tool, a total of 44 atomic concept questions developed by the American Association for Advancement of Science (AAAS) were translated and used. All questions in AAAS are multi-choice questions consisting of scientific concepts and misconceptions that students can have. This was put into 641 middle and high school students in Korea to measure the level of conceptual understanding of the state of atoms, molecules, and substances and compare it with the response rate of middle and high school students in the United States. As a result, high school students had a relatively higher rate of choosing correct answers than middle school student. The correct answer rate of Korean students was similar to that of American students, and Korean students also showed a high choice rate for wrong answers that American students showed a high choice rate. It was found that students in the two countries had similar misconceptions.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **EDU.P-459**
Chemistry Education
Exhibition Hall C FRI 11:00~13:00

Study on the impact of epistemological beliefs about scientific knowledge on teachers' personal knowledge

Seounghey Paik*, Kihyang Kim[1]

Department of Chemical Education, Korea National University of Education, Korea
[1]*Chemistry, Sejong Academy of Science and Arts, Korea*

This study aims to investigate the impact of science teachers' epistemological beliefs about scientific knowledge on their personal knowledge in the context of the concept of redox. Furthermore, the pedagogical effectiveness of a training program for changing epistemological beliefs about scientific knowledge was investigated. This study used questionnaires and interviews to reveal teachers' personal knowledge about the relationship between different redox models and to recognize the limitations of their personal knowledge by causing unexplained cognitive conflicts. The study also examined the process of cognitive conflict resolution of personal knowledge by introducing Goodstein's redox model and the process of change in perception of scientific knowledge. The results show that teachers' personal knowledge is influenced by their epistemological beliefs about scientific knowledge and affects how they present science to students during their teaching activities. Beliefs that scientific knowledge is derived from empirical entities, such as physical substances, were a barrier to accepting scientific concepts that were formed from abstract concepts and had the potential to convey misconceptions to students.

Poster Presentation : **ENVR.P-427**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Photophysical properties of a novel microplastic dye based on aggregation induced emission (AIE)

Jae Jun Lee, Hyejin Nam, Cheal Kim*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

A novel dye (B) was developed specifically for staining microplastics. Its unique photophysical properties, including solvatochromism and aggregation-induced emission (AIE), were corroborated via spectroscopic investigations. Solvatochromism analysis for B exhibited bathochromic shifts with increasing solvent polarity. Also, B showed a strong red fluorescence enhancement as the amount of water increased, which supported the AIE phenomenon of B. The stained microplastics and non-plastics with B were observed under a fluorescence microscope. Significantly, B was more selective in staining microplastics than non-plastic materials. B demonstrates superior cost advantages compared to Nile Red (NR), which is frequently employed for microplastic staining, owing to its uncomplicated synthesis process and great production efficiency. 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 : **ENVR.P-428**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

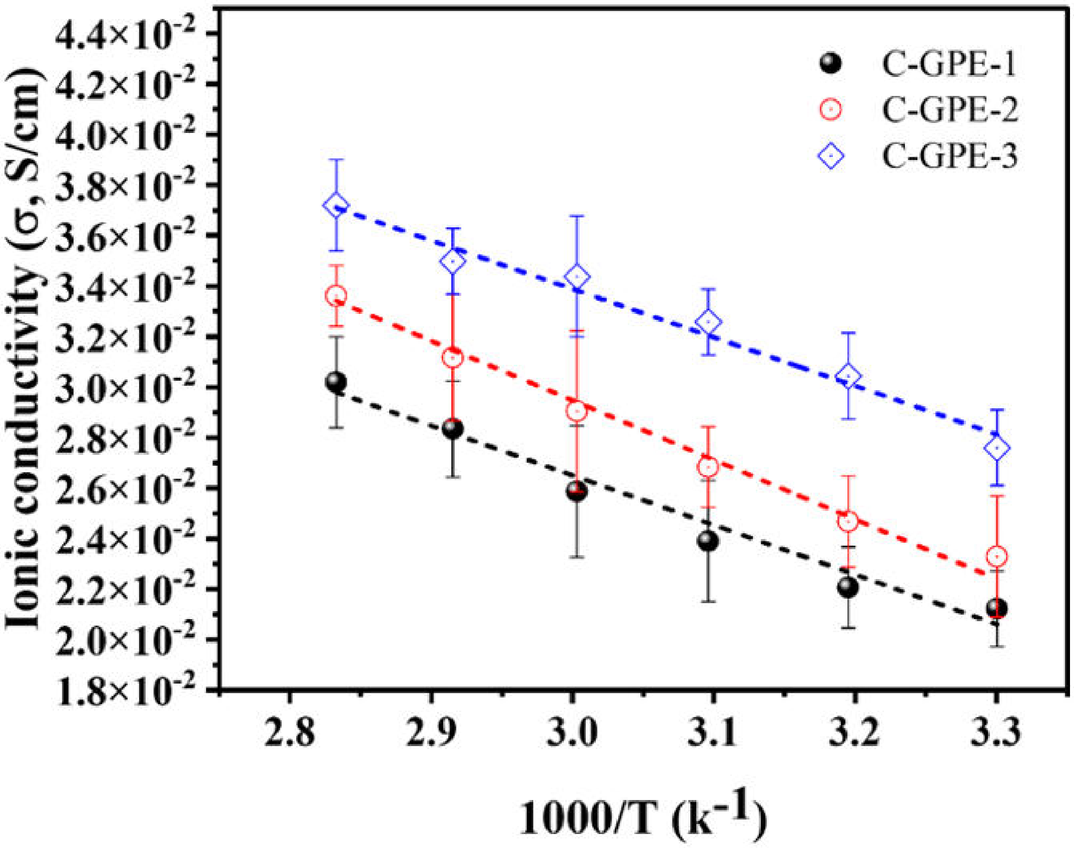
Study of Crosslinked Gel Polymer Electrolyte based on Epoxidized Soybean Oil and Lithiumbis(fluorosulfonyl)imide (LiFSI) for High-performances of Li-Ion Batteries

Wansu Bae, Minhyuk Jeon[1,*], Sungjun Park[*], Hohyoun Jang[*]

Applied Chemistry, Konkuk University, Korea

[1]Applied chemistry, Konkuk University, Korea

Unlike liquid electrolytes, which exhibit high ionic conductivity and a stable interface between the electrolyte and electrode, low ionic conductivity and an unstable electrolyte/electrode interface are significant obstacles that impede the advancement of lithium-ion batteries (LiBs) in practical applications. This research endeavors to address these challenges by developing a cross-linked gel polymer electrolyte (C-GPE) utilizing epoxidized soybean oil (ESO) as its base material. The synthesis involves in situ thermal polymerization, employing lithium bis(fluorosulfonyl)imide (LiFSI) as the initiator. Furthermore, the incorporation of ethylene carbonate/diethylene carbonate (EC/DEC) proves advantageous in enhancing the distribution of the prepared C-GPE on the anode surface and facilitating the dissociation ability of LiFSI. The synthesized polymer undergoes analysis through techniques such as Fourier Transform Infrared (FT-IR) spectroscopy, Thermogravimetric Analysis (TGA), and Differential Scanning Calorimetry (DSC) to evaluate its properties. Subsequently, the performance of the battery is assessed via a charge-discharge test to gauge its efficiency.



Ionic conductivity (σ, S/cm)
4.4×10⁻²
4.2×10⁻²
4.0×10⁻²
3.8×10⁻²
3.6×10⁻²
3.4×10⁻²
3.2×10⁻²
3.0×10⁻²
2.8×10⁻²
2.6×10⁻²
2.4×10⁻²
2.2×10⁻²
2.0×10⁻²
1.8×10⁻²
2.8
2.9
3.0
3.1
3.2
3.3
1000/T (k⁻¹)
C-GPE-1
C-GPE-2
C-GPE-3

Poster Presentation : **ENVR.P-429**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

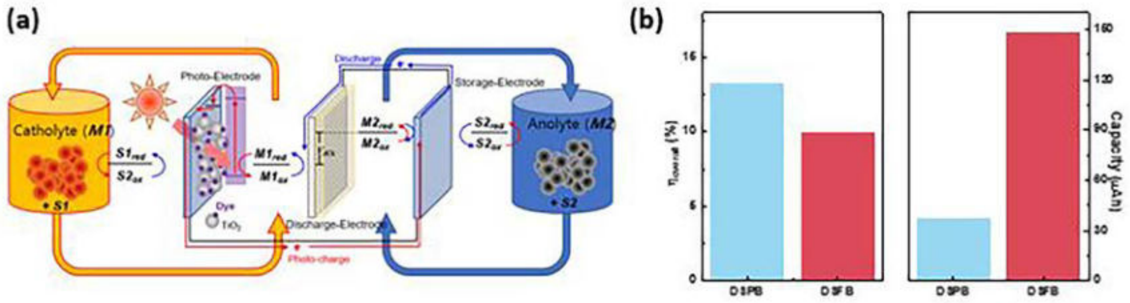
Development of Dye-Sensitized Photo-Rechargeable Flow battery for indoor light recycling

So Yeon Yoon, Tae-Hyuk Kwon[1,*]

department of chemistry, Ulsan National Institute of Science and Technology, Korea

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

Recently, with the increase in the use of wireless sensors and Internet-of-things(IoT) systems in daily life, the demand for battery used as power sources is rapidly increasing. However, batteries have to be replaced or recharged by grid electricity after their stored energy gets exhausted. In order to overcome these limitations, batteries that can be recharged using light energy used in daily life are being developed. As a previous study, dye-sensitized photo battery(DSPB) in which a dye-sensitized solar cell and a lithium battery were combined was reported and showed energy conversion efficiency of over 10 % under 1000 lux conditions(dim-light). DSPB is the first monolithic system for low light condition. Nevertheless, its small capacity limits its practical use. For this reason, we developed an integrated system with flow battery that is useful to increase capacity. For successful operation, we studied the mechanism of photo-charge. Then, for increasing solar to energy efficiency and capacity, we applied solid active materials. As a result, capacity increase 10 times compared to the previous study and the efficiency achieved about 10 %.


(a)
Catholyte (M1)
S1red
S2ox
• S1
Photo-Electrode
Dye
TiO2
M1red
M1ox
Discharge
Storage-Electrode
M2red
M2ox
S2red
S2ox
Anolyte (M2)
• S2
Discharge-Electrode
Photo-charge
(b)
η overall (%)
0
5
10
15
DSPB
DSFB
Capacity (μAh)
0
30
60
90
120
150
DSPB
DSFB

Poster Presentation : **ENVR.P-430**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Reduced TiO2 with serial treatment for electrochemical wastewater treatment.

Miao Wang, Hyunwoong Park*

School of Energy Engineering, Kyungpook National University, Korea

Recent studies have explored using titanium dioxide as an electrocatalyst to cure organic pollutants, particularly in wastewater. As one of the main topics for the reduced titanium dioxide, oxygen vacancies are formed during the hydrothermal treatment of titanium dioxide, which leads to a reductive state with a high potential for electrical conductivity. In a phosphate buffer solution, electrochemical reduction, thermal treatment of hydrogen gas, and sodium borohydride reduction were all investigated in this research. The impacts of various treatment procedures are contrasted by comparing the electrochemical effectiveness of the chlorine evolution process, the electrochemical stability assessment and analysis, the specific surface area, and other surface evaluations of the electrodes. Through these detailed comparisons, we offer the most rational advice and the most up-to-date perspectives for the reduction treatment of titanium dioxide in terms of electrocatalytic effectiveness, financial benefits, and environmental concerns.

Poster Presentation : **ENVR.P-431**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Fluorescent staining reagent capable of detecting plastics

Chanwoo Song, Jae Jun Lee[1], Cheal Kim[1,*]

Department Fine Chemistry, Seoul National University of Science & Technology, Korea

[1]*Department of Fine Chemistry, Seoul National University of Science & Technology, Korea*

Plastics, due to slow decomposition and inherent toxicity, pose a significant threat to marine ecosystems and human health. We synthesized BDB, a fluorescence staining reagent that has affinity to plastics in water, by combining an Aggregation-Induced Emission (AIE) active molecule with a fluorophore. A red-shift tendency according to the polarity of the solvent was verified through a solvatochromism test. As the water content increased, the AIE effect was observed. Therefore, BDB exhibited long-wavelength fluorescence in water. The staining experiments by using BDB were performed with various plastics and showed to detect them through red fluorescence change. 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 : **ENVR.P-432**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

AIE-based fluorescence staining reagent of various microplastic

Cheal Kim*, Hyejin Nam, Jae Jun Lee

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Plastics are very useful and mass-produced, but they make a lot of waste. The plastic debris becomes microplastic by weathering. Because microplastics cause enormous damage to the marine environment and harms organism, the detection of microplastics is important. In this work, a new staining method was chosen for easy and cheap detection of microplastics. Newly synthesized compound P1 has aggregation-induced emission (AIE) character so that P1 can stain microplastics by absorbing to microplastics. The AIE character is recognized by change of fluorescent intensity with variation of water-to-DMSO ratio and by Tyndall effect test. 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 : **ENVR.P-433**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Water splitting over Co/Ni-stainless steel electrodes

Seon Young Hwang, Juyoung Maeng, Choong Kyun Rhee, Youngku Sohn*

Department of Chemistry, Chungnam National University, Korea

The production of hydrogen and oxygen through water electrolysis has emerged as a compelling alternative to fossil fuels, capturing considerable interest. In this study, we employed a cobalt and nickel-co-electrodeposited stainless steel electrocatalyst to showcase its proficiency in facilitating both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Our main focus was on optimizing the performance of these essential reactions. Furthermore, we assessed the HER and OER performances using different feed gases, namely N_2, CO_2, and CO. The efficacy of these enhanced electrodes was comprehensively analyzed using various electrochemical techniques, encompassing electrochemical surface area measurements and Tafel plots. Additionally, spectroscopic methods including scanning electron microscopy, X-ray photoelectron spectroscopy, and energy-dispersive X-ray spectroscopy were employed to probe their fundamental physicochemical properties.

Poster Presentation : **ENVR.P-434**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Novel fluorescent dye for the detection of various microplastics

Boeun Choi, Cheal Kim*, Jae Jun Lee

Department of fine chemistry, Seoul National University of Science & Technology, Korea

Microplastics (MPs) not only cause environmental pollution but also have a very harmful effect on human health as they are generated and consumed in daily life. Therefore, a method to easily detect MPs is needed. Herein, we report the synthesis of a novel staining reagent and application for microplastics staining. DA emits red fluorescence and has the merits of being able to have low autofluorescence, photon scattering, and excitation energy. Eight types of MP were successfully stained. All MPs are quantified through ICY software. These results not only make it easy to detect harmful MPs but also provide good inspiration for developing new methods. 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 : **ENVR.P-435**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Electrochemical syngas production over Au/SrTiO3 electrodes

<u>Soyoung Kim</u>, Juyoung Maeng[1], Seon Young Hwang[1], Choong Kyun Rhee, Youngku Sohn[*]

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

Syngas, consisting of carbon monoxide (CO) and hydrogen (H2), has conventionally played a pivotal role in the synthesis of liquid fuels using Fischer-Tropsch (F-T) reactions, typically carried out through energy-intensive methods involving coal, natural gas, or biomass. This study provides a novel perspective by demonstrating the efficient electrochemical conversion of CO2 into syngas, facilitated by an Au-loaded SrTiO3 perovskite catalyst. Through careful adjustments of parameters such as Au overlayer thickness, applied potential, electrolyte composition, and concentration, precise control over the CO to H2 ratio in the resulting syngas is achieved, offering promising avenues for sustainable fuel production.

Poster Presentation : **ENVR.P-436**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Plastic staining application of a new dye with aggregation-induced emission

Soo Seong Lee, Jae Jun Lee, Chanwoo Song, Cheal Kim*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

The photophysical properties of a new fluorescent dye (1) were investigated through fluorescence spectrophotometry and UV-vis spectroscopy. 1 showed a novel aggregation-induced emission (AIE) property unlike typical AIE molecules. It exhibited a strong green fluorescence enhancement as the amount of water decreased. Also, the mechanofluorochromic (MFC) properties of 1 supported its novel characteristic of AIE. Solvatochromism analysis for 1 exhibited bathochromic shifts on increasing solvent polarity. Moreover, 1 could be successfully applied to stain various plastic samples in EtOH/DW mixture. 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 : **ENVR.P-437**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Electrochemical CO_2 conversion over Cu alloy composite oxide nanostructures

Ho Seong Yang, Seon Young Hwang, Juyoung Maeng, Choong Kyun Rhee, Youngku Sohn*

Department of Chemistry, Chungnam National University, Korea

The study investigates the electrochemical conversion of CO_2, employing surface treatment and alloy modification techniques on copper alloys. These alloys underwent a two-step process involving chemical oxidation followed by thermal treatment. The resulting composite oxide nanostructures of the alloys were subjected to evaluation under diverse conditions, including variations in electrolyte composition, concentration, and applied potential. The reduction products obtained were quantified using gas chromatography and nuclear magnetic resonance spectroscopy. The characteristics of the copper alloy composite oxide nanostructures were corroborated through scanning electron microscope and X-ray photoelectron spectroscopy.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ENVR.P-438**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Comparative Analysis of CuNiZn and CuZn Electrocatalysts for CO_2 Reduction

Yunji Kwon, Juyoung Maeng[1], Seon Young Hwang, Gaeun Yun[1], Choong Kyun Rhee, Youngku Sohn[*]

Department of Chemistry, Chungnam National University, Korea

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

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. Transition metal-based catalysts, such as copper-nickel-zinc (CuNiZn) and copper-zinc (CuZn) alloys, have shown potential for catalyzing CO_2 reduction reactions. Prominent reduction products, including H2, CO, CH_4, formate, and oxygenated hydrocarbons, were identified and verified through gas chromatography and nuclear magnetic resonance spectroscopy. These outcomes were then contextualized alongside Faraday efficiency, impedance, electrochemically active surface area, and fundamental physicochemical properties. Characterization techniques include X-ray photoelectron spectroscopy and energy-dispersive X-ray spectroscopy.

Poster Presentation : **ENVR.P-439**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Electrochemical CO_2 Conversion over electrodeposited Zn on Cu

Soo yeon Bae, Juyoung Maeng, Seon Young Hwang, Choong Kyun Rhee[1], Youngku Sohn[1,*]

Chemistry, Chungnam National University, Korea

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

Carbon dioxide (CO_2) recycling stands as a significant energy solution strategy. In this study, we utilized Cu electrodeposited with Zn to investigate electrochemical CO_2 conversion across various experimental parameters including electrolyte nature, concentrations, and applied potentials. The resulting CO_2 conversion products were characterized through gas chromatography and nuclear magnetic resonance spectroscopy. Additionally, we probed the underlying characteristics of the electrodes through scanning electron microscopy, X-ray photoelectron spectroscopy, and energy-dispersive X-ray spectroscopy. Furthermore, measurements of the electrochemically active surface area and impedance were also conducted.

Poster Presentation : **ENVR.P-440**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Electrochemical water splitting and CO_2/CO conversion over electrodeposited Cu on Ni foam

Gaeun Yun, Seon Young Hwang, Choong Kyun Rhee, Youngku Sohn*

Department of Chemistry, Chungnam National University, Korea

Electrochemistry presents highly promising solutions for addressing energy and environmental challenges, particularly in the realm of energy production and storage. In this study, our focus was directed toward the development of electrodeposited copper on nickel foam, and we scrutinized its performance in various electrochemical processes such as CO_2/CO conversion and water splitting. Additionally, an experiment was conducted using electrodeposited nickel on copper foam, and the outcomes were subsequently compared. We contrasted the effects of hydrogen evolution reaction and the oxygen evolution reaction. Furthermore, we conducted an examination of the surface elemental oxidation states using X-ray photoelectron spectroscopy.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

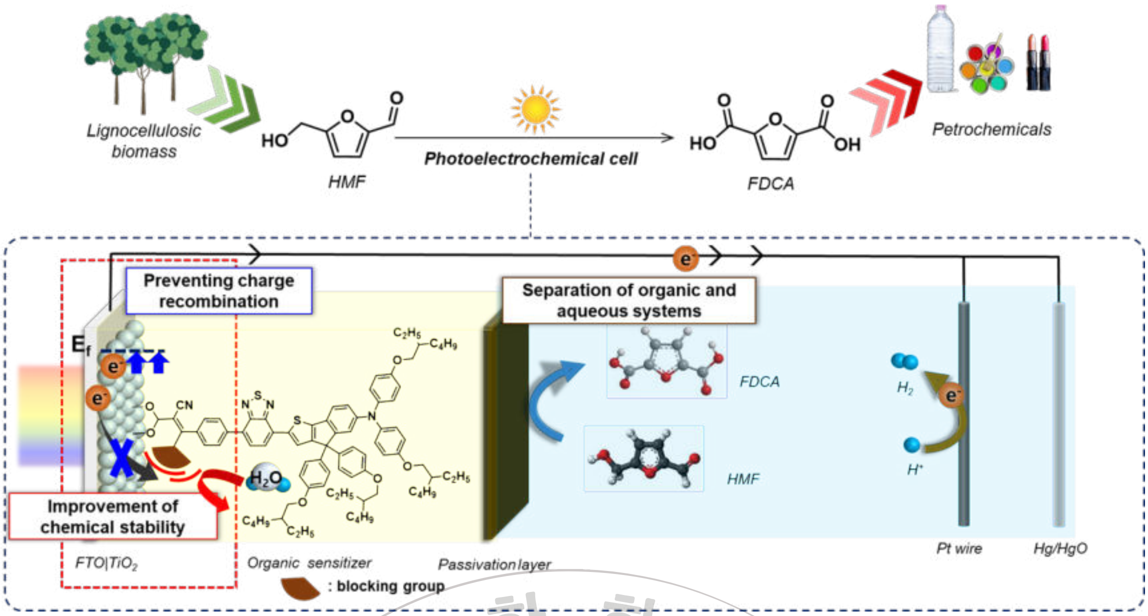
Poster Presentation : **ENVR.P-441**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Photo-electro-upcycling of biomass via dye-sensitized photoanode with passivation effect

Jeong Kyeong Lee, Tae-Hyuk Kwon[1,*], Deok-Ho Roh[1], So Yeon Yoon[2]

Ulsan National Institute of Science and Technology, Korea
[1]Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[2]department of chemistry, Ulsan National Institute of Science and Technology, Korea

Solar valuable chemical conversion is being actively studied for a sustainable environment. Organic dye-sensitized semiconductor systems are suitable due to their easy band gap tuning, broad absorption spectrum, facile fabrication, and relatively low priced compared to metal complexes to convert light to valuable substances effectively and stably. However, charge transfer from biomass to oxidized organic dye is relatively slow in typical dye-sensitized photoelectrochemical cells, resulting in remarkably low current density, unlike photovoltaics. Hence, the holes can be extracted from organic dye-sensitized photovoltaic system with passivation effect enhancing its efficiency and they can directly oxidize biomass. Organic dyes are researched to generate high current and voltage related to conversion yield and selectivity, so we designed IDT-1−4 organic dyes. Significantly, the methyl functional group is introduced to the acceptor unit to prevent loss of the photovoltage through slow recombination from TiO2 to oxidized organic dyes. This study shows that biomass can be oxidized and degraded with low applied bias and relatively short time.


Lignocellulosic biomass
HO
O
O
HMF
Photoelectrochemical cell
HO
O
O
O
OH
FDCA
Petrochemicals
e
Preventing charge recombination
Separation of organic and aqueous systems
E_f
e
e
CN
O
O
S
N
N
S
N
O
C_2H_5
C_4H_9
H_2O
O
O
O
C_2H_5
C_4H_9
C_4H_9
C_2H_5
C_4H_9
C_2H_5
X
FDCA
HMF
H_2
e
H^+
Improvement of chemical stability
FTO|TiO_2
Organic sensitizer
Passivation layer
: blocking group
Pt wire
Hg/HgO

Poster Presentation : **ENVR.P-442**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

An aggregation-induced emission-based fluorescence micro-plastic probe using staining function

Yun-Seo Lee, Cheal Kim*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

We made an aggregation-induced emission (AIE) based micro-plastic probe 1 to detect micro-sized plastics by staining method. The solvatochromism of probe 1 displayed bathochromic shift using spectroscopic study caused by polarity effects. An emission spectrum and the image of tyndall effect were shown to back up the AIE effect. Various micro-plastics and non-plastics were dyed with the probe 1 in a near perfect aqueous solution. Unlike non-plastics, the green fluorescence of all plastics was emitted by staining process. Therefore, probe 1 was demonstrated as a micro-plastic probe selectively and efficiently. 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).

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ENVR.P-443**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Enhanced properties of bismuth oxyhalides (BiOX X = Cl, Br, I)/RGO heterojunction for sustainable applications

Ga Hyeon Ha, Taeho Shin[1,*]

Dynamics & Spectroscopy / Carbon Composites Convergence Materials Engineering, Jeonbuk National University, Korea

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

In this study, we present a novel heterogeneous photocatalyst synthesized via a facile hydrothermal method aimed at addressing global environmental challenges and energy scarcity. Bismuth oxyhalides (BiOX, where X = Cl, Br, and I) were chosen as the basis for their cost-effectiveness and distinctive layered structures, making them popular choices for photocatalysis. However, the photocatalytic efficacy of BiOX materials is often hindered by rapid charge carrier recombination. To surmount this limitation, a heterojunction structure was engineered by integrating reduced graphene oxide (RGO) due to its strong electrical conductivity and visible light absorption capabilities. Comprehensive characterization involving field emission scanning electron microscopy (FE-SEM), UV-visible diffuse reflectance spectra (DRS), X-ray diffraction (XRD), and Brunauer-Emmett-Teller (BET) surface area analysis was performed to elucidate the morphology, optical properties, and structure of the BiOX/RGO composites. The distinctive BiOX/RGO composites exhibited augmented visible light absorption, attributed to their substantial specific surface area, resulting in a notable enhancement of their photocatalytic performance. Particularly, the most efficient composite, BiOCl/RGO, demonstrated nearly complete degradation of 99% of methylparaben (MEP) at a concentration of 300 mg/L. Additionally, a comprehensive toxicity assessment was conducted to evaluate the composite's impact on both microbial and phytosystems.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ENVR.P-444**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Spectroelectrochemical Study of the Local Environment of CO_2 to CO Conversion on Nanostructured Electrode using In Situ ATR-SEIRAS

Bupmo Kim, Wooyul Kim*, Wonyong Choi*

Institute for Environmental and Climate Technology, Korea Institute of Energy Technology (KENTECH), Korea

In this manuscript, we investigated the intrinsic electrochemical behavior that occurs on catalytic surfaces during the conversion of CO_2 to CO, focusing on the nanostructured-porous Au electrode. We used a high-temperature non-aqueous anodization process to fabricate the nanosponge Au electrode and revealed that the Au-nanosponge showed higher current density and faradaic efficiency for CO production than the flat Au electrode, which was attributed to the different local electric environment. Thus, to monitor the reaction intermediates and local chemicals, in situ surface-enhanced infrared absorption spectroscopy (SEIRAS) was conducted. The main findings of this study include that the nanoporous Au electrode has a dominant active site, promoting the linear CO intermediate and suppressing the bridging CO intermediate when compared with the non-structured Au electrode. Furthermore, we also revealed a high local pH at a reaction potential of -0.9 V (vs. RHE), and the slow diffusion kinetics of local CO_3^{2-} at an open circuit potential. This study is significant because it provides important insights into the electrochemical CO_2 reduction process and can contribute to the development of more efficient and cost-effective electrocatalysts for CO_2 reduction.

Poster Presentation : **ENVR.P-445**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Advances in Photoelectrochemical Systems for Enhanced and Selective Glycerol Oxidation

HoSub Bae, Wonyong Choi[1,*]

Environmental Science & engineering, Pohang University of Science and Technology, Korea
[1]*Institute for Environmental and Climate Technology, Korea Institute of Energy Technology (KENTECH), Korea, Korea*

Glycerol oxidation holds significance as it offers a pathway to transform a readily available byproduct into value-added chemicals, contributing to sustainable resource utilization. Additionally, enhancing the selectivity of glycerol oxidation reactions can lead to the production of valuable compounds with diverse applications in industries such as pharmaceuticals and fine chemicals. One promising approach is photoelectrochemical (PEC) solar fuel production, which transforms renewable solar energy into valuable products. This research aims to improve glycerol's selectivity towards dihydroxyacetone by modifying the TiO_2 nanorods photoanode. We successfully created the TiO_2 nanorods photoanode and introduced modifications using an organic polymer (CN) with O and P elements (CNOP). For hydrogen peroxide production, single-walled carbon nanotube (CNT) electrodes with anchored anthraquinone (AQ-CNT) were used at the cathode. Importantly, the system maintained stability throughout durability testing and recycling experiments, demonstrating its robustness. This study highlights the potential of the unassisted PEC system for sustainable energy conversion and chemical synthesis, showcasing its promise for creating valuable products at both electrodes. These findings contribute to the global push for a greener future through advanced solar fuel production methods.

Poster Presentation : **ENVR.P-446**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Cyclodextrin loaded WO_3 for successful utilization of visible light in volatile organic compounds (VOCs) degradation

Woojung Jeon, Wonyong Choi[1,*]

Chemical Engineering, Pohang University of Science and Technology, Korea

[1]*Institute for Environmental and Climate Technology, Korea Institute of Energy Technology (KENTECH), Korea*

For a sustainable and pollution-free photochemical air purification system, visible-light-driven photocatalyst, especially WO_3, activated by natural light is under intense investigation. We employed carboxymethyl-β-cyclodextrin (CMCD), which is an oxygen-rich carbon material, as a co-catalyst to replace noble metals (especially Pt), prepared CMCD-loaded tungsten trioxide (CMCD/WO_3), and demonstrated its highly enhanced VOCs degradation activity. CMCD/WO_3 showed ~15 times higher acetaldehyde mineralization efficiency than bare WO_3, which is comparable to Pt-loaded WO_3. The enhanced acetaldehyde removal efficiency with a near-stoichiometric conversion to CO_2 eliminates the risk of secondary pollution by minimizing the intermediate generation. Oxygen-rich carbonaceous CMCD-loaded WO_3 was able to remove acetaldehyde while maintaining its activity even under low oxygen conditions. On the other hand, in the absence of H_2O, the photocatalytic activity was remarkably hindered, which means CMCD/WO_3 produces OH radicals through the direct hole oxidative pathway dominantly with or without oxygen. Anchoring food-grade cyclodextrin onto WO_3 provided hydrophilic outer surface to adsorb atmospheric moisture rapidly, resulting in further activating the H_2O oxidative pathway. OCVD profiles proved anchored CMCD captures more electrons in this oxygen-rich macrocylic ring structure. Therefore, the lifetime of the charge carriers becomes longer and the more holes efficiently react with adsorbed water molecules. CMCD as a carbonaceous co-catalyst is a unique candidate to replace expensive noble-metal for air purification.

Poster Presentation : **ENVR.P-447**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Development of VOCs Filter Utilizing Simultaneous Functions of Adsorption by Ion Exchanger and Photodegradation by Photocatalyst

Yungyoon Kim, **Wonyong Choi**[1,*]

Institute for Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

[1]*Chemical, Environmental & Climate Technology Laboratory, Korea Institute of Energy Technology (KENTECH), Korea*

With the growing concern about global air pollution, the industrial sector and households are increasingly interested in indoor air quality. Indoor air pollution has various causes, but volatile organic compounds (VOCs) are the most prominent. VOCs' primary human health risks include respiratory issues, neurological effects, and potential carcinogenicity.The current VOCs filter market is predominantly dominated by activated carbon materials, with ion exchange filters being utilized in conjunction. However, these materials' drawbacks are the incurred post-processing costs and the potential for causing additional environmental contamination. In response, we have conceived a novel filter design. In my previous research, I observed that the affinity between the target VOCs and the ligands used in ion exchange could be reduced, allowing the material to be released over time. Utilizing this characteristic, we have devised a design incorporating ion exchange adsorption functionality on the front and a photocatalyst on the rear.Through the adsorption capabilities of the ion exchange part, the initial concentration of target VOCs is rapidly reduced, followed by the degradation of VOCs through the photocatalyst. As time elapses, ligands with weak binding with VOCs are expected to release adsorbed VOCs, enabling a process in which the photocatalyst can subsequently degrade them once again. Through this design, it is expected that a material capable of overcoming adsorption saturation limits and the time required for photocatalyst deactivation processes can be created.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

Poster Presentation : **ENVR.P-448**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Interface engineering of TMDs and CoP heterostructure on Carbon cloth for highly efficient hydrogen evolution reaction

Sohyeon Hong, Sunny Park, Ye Joo Kwon, Soo Min Kim*

Chemistry, Sookmyung Women's University, Korea

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.

Poster Presentation : **ENVR.P-449**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Gold (III) recovery and reduction from complex matrices using thiol functionalized MOFs.

Luis Mario Rendon, Hasan Fareed[1], Seunghee Han[2,*]

ENVIRONMENTAL, GIST, Korea

[1]*School of Earth Science and Environmental Engineering, Gwangju Institute of Science and Technology, Korea*

[2]*School of Environmental Sciences and Engineering, Gwangju Institute of Science and Technology, Korea*

The creation of proficient adsorbents for the recovery of precious metals from secondary resources is of great environmental and economic significance. In this study, an effective Metal-Organic Framework (MOF) UiO-66-NH2-DMTD made up by modifying Zr-MOF (Zirconium-based Metal-Organic Framework) with 2,5-Dimercapto-1,3,4- thiadiazole (DMTD) has been proposed as a promising redox-active catalyst capable of recovering gold (Au) from complex liquid matrices, including microwave-digested incinerated bottom ash (IBA), Han River water, digested CPU processor, and simulated wastewater matrices using deionized water. It is suggested that the recovery of Au (III) nanoparticles onto UiO-66-NH2-DMTD is irreversible, due to a chemisorption process confirmed through the Langmuir isotherm and pseudo-second-order model. UiO-66-NH2-DMTD shows an extraordinary experimental adsorption capacity that reaches an estimate of 878.5 mg g−1 at a pH of 3.0 and 338 K. Outstandingly, it has a high ability to selectively and effectively capture Au (III), even when coexisting ions are present at concentrations 5 times higher in Han River water. This exceptional selectivity is attributed to a combination of electrostatic interactions, coordination, and reduction mechanism’s reaction between Au (III) and the sulfide group encompassed in the DMTD functional groups. Remarkably, it was verified that the reduction of Au (III) to metallic gold was a dominant recovery mechanism. Moreover, the recyclability and recovery tests demonstrated the potential for the catalyst to be reused displaying notable

stability, enhancing its practical applicability, with its adsorption performance showing only minimal reduction recovery rates even after undergoing 12 recycling processes. Furthermore, the industrialized application of the MOF was observed in experiments involving liquid matrices with leached Au, Cu, and Ni extracted from a CPU processor, incinerated bottom ash, and river water, highlighting the current practical viability of UiO-66-NH2, particularly with its DMTD ligand functionalized into the parent structure. These results collectively demonstrated that the UiO-66-NH2-DMTD was an effective sustainable adsorbent for the efficient and selective recovery of Au (III) in complex liquid matrices.

Poster Presentation : **ENVR.P-450**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Enhanced Adsorption of Chromium(VI) onto Microplastics via Freeze-Concentration Effect in Heterogeneous Aquatic Environments

Hyuncheol Kim, Bomi Kim, Kitae Kim[1,*]

Research Unit of Cryogenic Novel Materia, University of Science & Technology, Korea Polar Research Institute School, Korea

[1]*Research Unit of Cryogenic Novel Materia, Korea Polar Research Institute, Korea*

Microplastics (MPs) adsorb various substances, such as organic pollutants or heavy metals like Cr(VI), impacting the environment and ecosystem. However, the short-term adsorption of Cr(VI) onto MPs in MP/water/pollutants in heterogeneous environments has rarely been investigated. This study focuses on the quantitative analysis of the increased Cr(VI) adsorption onto MPs through freezing on a relatively short-term scale. The experimental results showed when the Cr(VI) solution was frozen without adding MPs, Cr(VI) was reduced by 51%. Conversely, when MPs were added, a reduction of 87% of Cr(VI) was achieved. This increased adsorption is attributed to the "freeze-concentration effect," where materials excluded from ice crystals during freezing accumulate at the "quasi-liquid layer (QLL)" within ice crystal boundaries. In the MP/water/pollutants heterogeneous system, the freeze-concentration effect made a cluster of MPs and Cr(VI) within the QLL, leading to increased adsorption of Cr(VI) onto MPs. A comparative analysis was conducted by the presence of MPs in the Cr(VI) solution, along with the distinctions observed between the aqueous phase and frozen phase.Raman spectroscopic study verified the concentrations of MPs and Cr(VI) within the QLL due to the freeze-concentration effect. DPC colorimetric method was used to monitor Cr(VI) concentration based on freezing and time, while TEM-EDS analysis confirmed Cr(VI) adsorption onto the surface of MPs. The result suggests a notable increase in Cr(VI) adsorption onto MPs during freezing, highlighting the potential of the freeze-concentration effect to enhance the adsorption of pollutants, such as Cr(VI), in various natural environments such as wintertime in a mid-latitude area, and polar regions.

Poster Presentation : **ENVR.P-451**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Suppressing salt transport through self-crosslinked MXene membranes for brine treatment by pervaporation

<u>Hasan Fareed</u>, Seunghee Han[1,*]

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

[1]*School of Environmental Sciences and Engineering, Gwangju Institute of Science and Technology, Korea*

MXene based 2D lamellar membranes suffer from notorious swelling issues which can be attenuated using various crosslinking agents thus ending up in expensive/cumbersome synthesis process. Additive free self-crosslinking technique was optimized based on dehydroxylation of MXene inherent functional groups to form Ti – O – Ti bond using thermal treatment explicitly tailored for pervaporative desalination of brine in this study. Ultra-thin (~100 nm) MXene membranes were synthesized using facile vacuum filtration technique and were crosslinked at different temperature range (25 – 180 °C) inspired from thermogravimetric analysis. XPS revealed Ti-O-Ti bond formation induced from dehydroxylation which helped in reduced and stable d-spacing resulting in increased surface roughness and water contact angle. M140 (Membrane crosslinked at 140 C) proved to be the optimized membrane in terms of permselectivity of water/salt mixture. Pervaporation results showed that M140 membrane generated permeation flux of 70 Kg m-2 h-1 with rejection upto 99.9 % for synthetic saltwater having 100g/L of NaCl at the feed temperature of 70 °C. Furthermore, M140 was tested for simulated brine (Mass ratio of Monovalent/Divalent salt = 6) for continuous 48 h of operation which showed successful suppression of salt transport on permeate side which was further confirmed by SEM analysis. M140 can be confidently recommended for pervaporation desalination where high salinity feed is expected.

132nd General Meeting of the Korean Chemical Society
October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ENVR.P-452**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Computation study on the thermodynamic energies of HyBRID dissolution reaction considering Cu-hydrazine complex formation

Jihun Oh, Young-Kyu Han*

Energy of Materials Engineering, Dongguk University, Korea

Decontamination is one of the important processes for dismantling nuclear power plants. The purpose of decontamination is to reduce the radiation levels of contaminated nuclear facilities, ensuring the safety of workers involved in decommissioning and minimizing the amount of radioactive waste. In this study, we investigate the reaction mechanisms and their thermodynamic energies of the HyBRID (Hydrazine-Based Reductive participated metal Ion Decontamination) process for decontamination of the primary coolant system of a nuclear power plant. We computed the thermodynamic properties of HyBRID dissolution mechanisms in which corrosion metal oxides accumulated in the primary coolant systems along with radionuclides are dissolved by HyBRID decontamination agents ($H_2SO_4/N_2H_4/CuSO_4$). The HyBRID reaction mechanism has been studied using a commercial database (HSC Chemistry®), but Cu ions have been used instead of Cu-hydrazine complexes when calculating reactions due to the absence of thermodynamic properties for Cu-hydrazine complexes. To address this limitation, we supplemented the quantum calculations with Cu-hydrazine complexes using the density functional calculations. It is intended to simulate a more practical reactions by calculating the reactions considering Cu-hydrazine complexes, and to improve understanding of the HyBRID dissolution reactions by qualitatively and quantitatively comparing the reactions without considering the complex formation.

132nd General Meeting of the Korean Chemical Society

October 25(Wed)~27(Fri), 2023, Kimdaejung Convention Center, Korea

---

Poster Presentation : **ENVR.P-453**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

Experimental study of the intrusive behavior of microplastics in ice via freezing-concentration

Bomi Kim, Hyuncheol Kim, Kitae Kim[1,*]

University of Science & Technology, Korea

[1]*Korea Polar Research Institute, Korea*

Microplastic pollution in the polar regions is an emerging environmental concern in the last decade. It is known that the microstructural environment in ice can interact with toxic chemical substances (including organic molecules and heavy metal ions) to attenuate their toxicity or transform them into more toxic substances. Therefore, determining the behavior of microplastics in ice is important to elucidate the mechanisms of pollution from microplastics in polar regions.In this study, polystyrene (PS) 1 um beads were used as a standard model of microplastics to study the freezing-concentration of microplastics following freezing temperature, salt concentration, microplastic concentration, and freezing method. After freezing the microplastic solution under different temperature conditions and freezing times, the ice cross-section was cut to a certain height and analyzed by stereomicroscopic images. The results showed that in the presence of salt, most of the microplastics were gathered into the microstructure of the ice, depending on the freezing rate. These experimental results suggest that freezing-concentration of microplastics in ice grain boundaries is more likely to occur in natural environmental conditions such as seawater, suggesting that microplastics present in polar environments may be more biotoxic due to the increased adsorption of chemical species in ice microstructure.

Poster Presentation : **ENVR.P-454**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

The role of poly siloxane-spacer in Y6 derivative acceptor copolymers of all-polymer solar cells for mechanical robustness

Yun Hi Kim[*], Bumjoon Kim[1,*], Jingwan Kim[2]

Department of Chemistry, Gyeongsang National University, Korea

[1]*Department of Chemical Engineering & Biotechnology, Korea Advanced Institute of Science and Technology, Korea*

[2]*Gyeongsang National University, Korea*

Organic solar cells (OSCs) have attracted research interest by their elastic character for wearable and stretchable devices. Especially all-polymer OSCs with same composition unit between donor and acceptor are enhanced their thermal stability and mechanical robustness. However, in most of OSCs, high elasticity often reduces the power conversion efficiency (PCE) by low charge transfer be cacused by weak aggregation of each donor and acceptor composite. In this study, new polymer acceptors consisted by the poly siloxane-spacer (PSS) with benzoditohiophene (BDT) and Y6 non-fullerene small molecule acceptor (NFSMA) derivative are synthesized and characterized for high performance and highly stretchable OSCs. The PSS unit has intrinsically stretchable property due to their rubber like structure, therefore introducing PSS unit as a building block in the OSC polymers suggests improve its own elasticity of the OSC polymers. In addition, introducing PSS unit increase solubility of OSC polymers, enabling high performance OSC by solution process using a non-halogenated green solvents. For example, all-polymer OSCs based on PSS containing polymer achieved more high PCE value (13.5 %) and crock-onset strain (COS = 15.2 %) than non-containing one (PCE = 9.8% and COS = 9.6%)

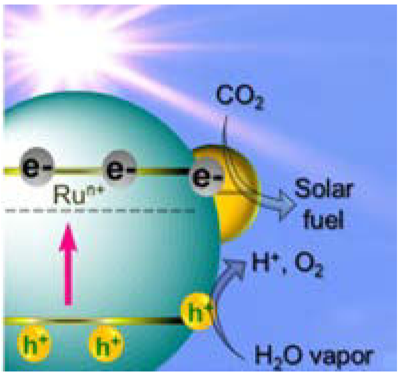
Poster Presentation : **ENVR.P-455**
Environmental Energy
Exhibition Hall C THU 11:00~13:00

Surface modified Ag@Ru-P25 for photocatalytic Carbon dioxide conversion with high selectivity over Methane formation at the solid–gas interface

Hwapyong Kim, **Su Il In**[1,*]

Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Systematic optimization of the photocatalyst and investigation of the role of each component is important to maximizing catalytic activity and comprehending the photocatalytic conversion of CO_2 reduction to solar fuels. A surface-modified Ag@Ru-P25 photocatalyst with H_2O_2 treatment was designed in this study to convert CO_2 and H_2O vapor into highly selective CH_4. Ru doping followed by Ag nanoparticles (NPs) cocatalyst deposition on P25 (TiO_2) enhances visible light absorption and charge separation, whereas H_2O_2 treatment modifies the surface of the photocatalyst with hydroxyl (–OH) groups and promotes CO_2 adsorption. High-resonance transmission electron microscopy, X-ray photoelectron spectroscopy, X-ray absorption near-edge structure, and extended X-ray absorption fine structure techniques were used to analyze the surface and chemical composition of the photocatalyst, while thermogravimetric analysis, CO_2 adsorption isotherm, and temperature programmed desorption study were performed to examine the significance of H_2O_2 treatment in increasing CO_2 reduction activity. The optimized Ag1.0@Ru1.0-P25 photocatalyst performed excellent CO_2 reduction activity into CO, CH_4, and C_2H_6 with a ~95% selectivity of CH_4, where the activity was ~135 times higher than that of pristine TiO_2 (P25). For the first time, this work explored the effect of H_2O_2 treatment on the photocatalyst that dramatically increases CO_2 reduction activity.


CO₂
e-
e-
e-
Ruⁿ⁺
Solar fuel
H⁺, O₂
h⁺
h⁺
h⁺
H₂O vapor

Poster Presentation : **ENVR.P-456**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

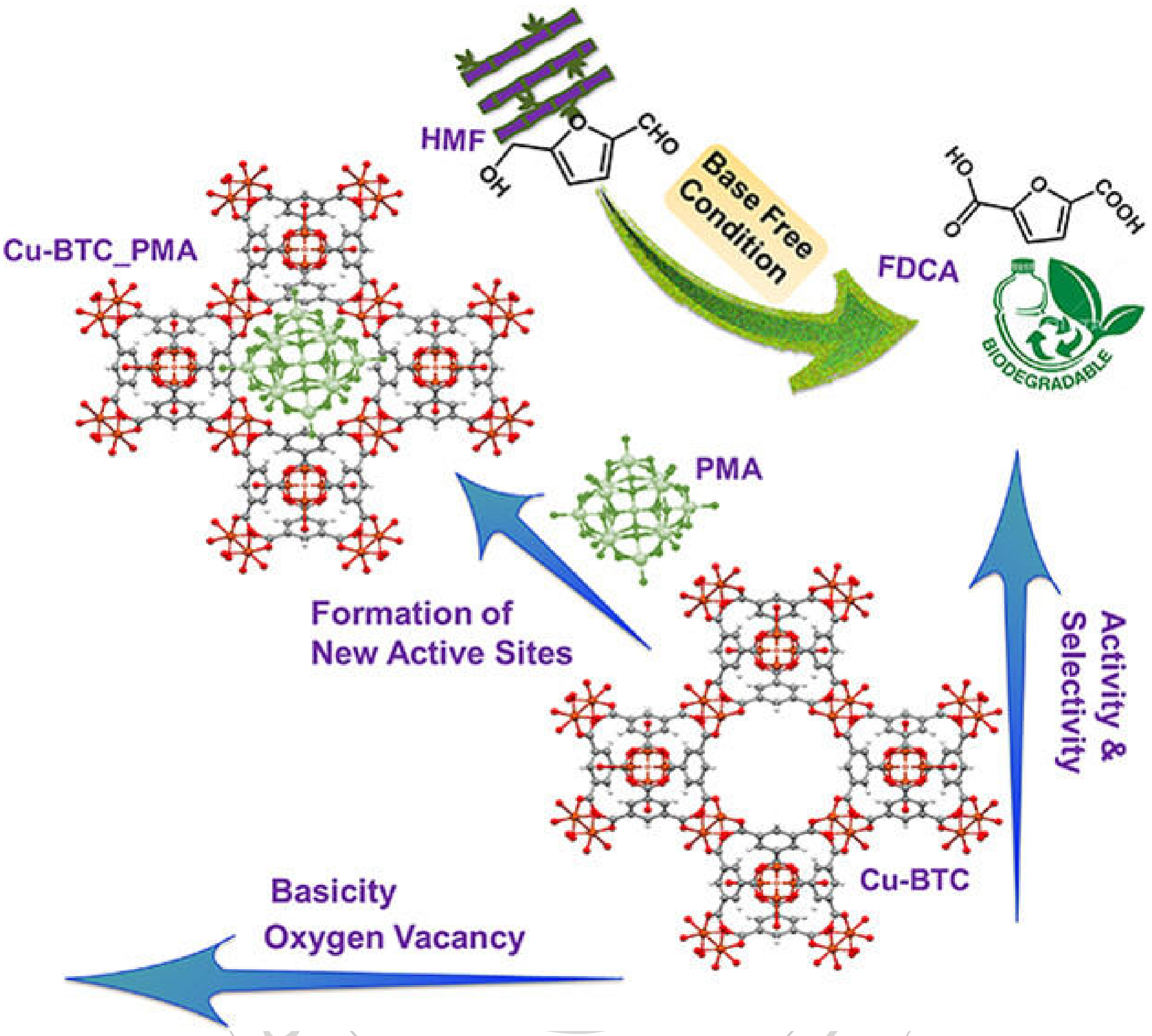
Elucidation of Active Sites and Mechanistic Pathways of a Heteropolyacid/Cu-Metal–Organic Framework (MOF) Catalyst for Selective Oxidation of 5-Hydroxymethylfurfural

Hwapyong Kim, **Su Il In**[1,*]

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

[1]*Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

5-hydroxymethylfurfural (HMF) oxidation into FDCA involves the concurrent oxidation of primary alcohol and an aldehyde functional group into carboxylic groups, which therefore demand a bifunctional catalyst containing dual active sites and chemoselective oxidation of HMF. The present work demonstrated the formation of new selective active sites in a composite porous material (Cu-BTC_PMA) that consists of Cu-BTC (metal–organic framework (MOF)) and polyoxometalate (POM). The porous framework provides (Cu-BTC_PMA) the desired chemoselectivity, while a selective Cu metal center in Cu-BTC (MOF) and Cu–O–Mo sites functions as active sites for the concurrent oxidation of HMF into FDCA. This catalyst exhibited a HMF conversion of 89% and an FDCA selectivity of 92.3% under base-free and mild reaction conditions. In detail, X-ray absorption spectroscopy analysis demonstrated the chemical bond tuning, as well as electronic structural modulations of MOF and POM at the molecular level, which directs the formation of new synergistic interfacial active sites and charge transfer states. This phenomenon causes the generation of the unique redox environment of copper and the multiple oxidation states along with the oxygen vacancy in the Cu-BTC_PMA catalyst, which most likely behaves as active sites for base-free oxidation.Moreover, we made comparative density functional theory and quantum theory of atoms in molecules investigations on the surface interaction between the reactant (HMF) and two catalyst models of Cu-BTC and Cu-BTC_PMA to interpret quantitatively the higher catalytic activity of the Cu-BTC_PMA catalyst. The kinetics study also evaluates the rate-determining step and activation energy for the multistep oxidation reactions.



Poster Presentation : **ENVR.P-457**

Environmental Energy

Exhibition Hall C THU 11:00~13:00

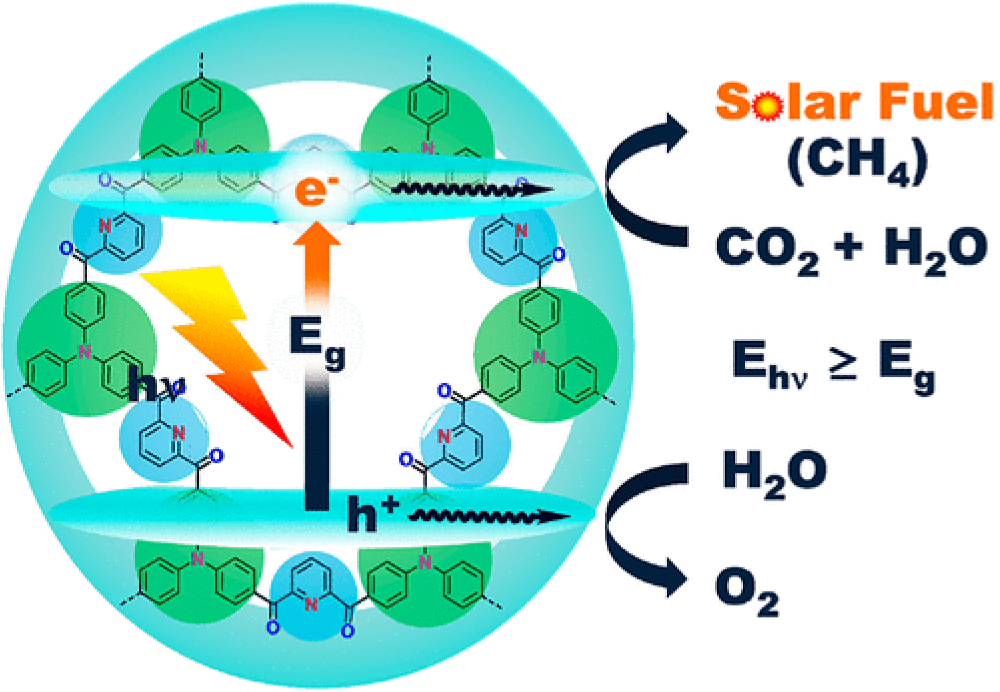
Nanoarchitectonics of Porous Polyketone without metal as Photocatalytic Assemblies for Artificial Photosynthesis

<u>Hwapyong Kim</u>, Su Il In[1,*]

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

[1]Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

The main component of natural gas is methane, whose combustion contributes to global warming. As such, sustainable, energy-efficient, nonfossil-based methane production is needed to satisfy current energy demands and chemical feedstocks. In this article, we have constructed a metal-free porous polyketone (TPA-DPA PPK) with donor–acceptor (D–A) groups with an extensive π-conjugation by facile Friedel–Crafts acylation reaction between triphenylamine (TPA) and pyridine-2,6-dicarbonyl dichloride (DPA). TPA-DPA PPK is a metal-free catalyst for visible-light-driven CO_2 photoreduction to CH_4, which can be used as a solar fuel in the absence of any cocatalyst and sacrificial agent. CH_4 production (152.65 ppm g–1) is ∼5 times greater than that of g-C_3N_4 under the same test conditions. Charge-density difference plots from excited-state time-dependent density functional theory (TD-DFT) calculations indicate a depletion and accumulation of charge density among the donor/acceptor functional groups upon photoexcitation. Most notably, binding energies from DFT demonstrate that H_2O is more strongly bound with the pyridinic nitrogen group than CO_2, which shed insight into mechanistic pathways for photocatalytic CO_2 reduction.


Solar Fuel
(CH4)
CO2 + H2O
Ehν ≥ Eg
H2O
O2
e-
Eg
hν
h+
N
O