Plenary Lecture : **PLEN-1**

Plenary Lecture

Convention Hall2 THU 13:00

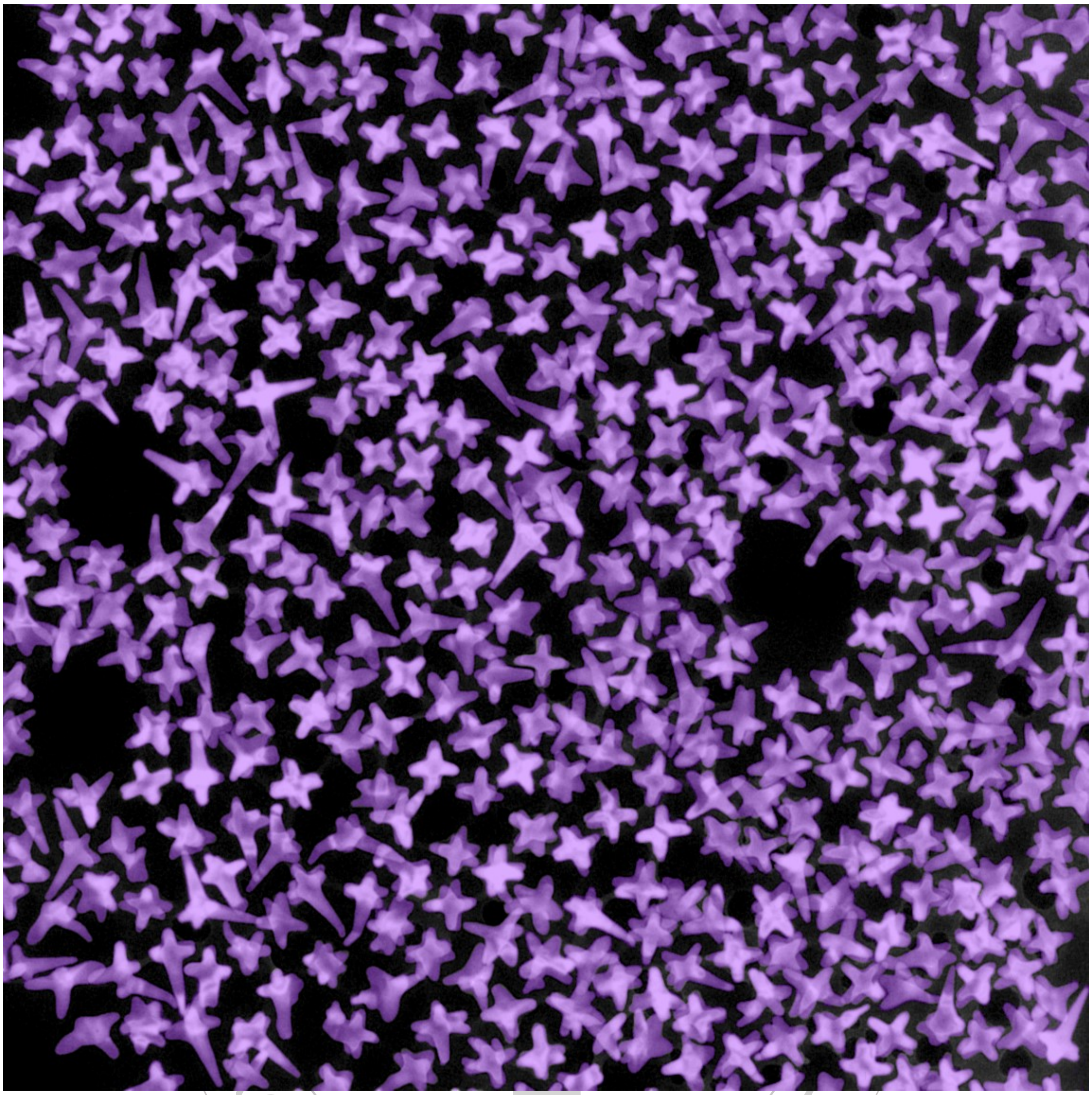
Chair: Jwa-Min Nam (Seoul National University)

Nanoparticle Shape Effects on Nano-Bio Interactions

Teri W. Odom

Northwestern University, United States

Anisotropic gold nanoparticles exhibit shape-dependent properties beneficial for drug delivery vehicles, imaging probes, and therapeutic agents. Although increased therapeutic efficacy has been realized, direct visualization of how engineered nanoparticles interact with specific organelles or cellular components has been limited. Such interactions will have implications for fundamentals in cancer biology as well as in the design of translational nanoconstructs. This talk will describe how drug-loaded gold nanostars can behave as optical probes to interrogate how targeting nanoconstructs interact with cells at the nanoscale. We will focus on model cancer cell systems that can be used to visualize how gold nanoconstructs target cells, rotate, and translate on the plasma membrane and are endocytosed and trafficked intracellularly. Differences in single-particle dynamics reveals how nanoparticle geometry affects binding to cell-membrane receptors and internalization. That nanoparticle shape can preserve ligand activity of nanoconstructs extracellularly as well as dictate spatial organization intracellularly will have important implications for engineering designer nanoconstructs for nanomedicine.



Plenary Lecture : **PLEN-2**

Plenary Lecture

Convention Hall2 THU 13:40

Chair: Jwa-Min Nam (Seoul National University)

Conformal Nano-bio Interfaces for Sense Digitalization

Xiaodong Chen

Innovative Centre for Flexible Devices (iFLEX), School of Materials Science and Engineering, Nanyang Technological University, Singapore

The rising demand for the interconnectedness of electronic devices and data science has led to a greater need for seamless human-electronic device integration. However, the major challenge lies in the inability of conventional electronics to pick up reliable biological signals from the human body. This is due to fundamental mismatches such as incompatible surfaces (soft skin vs rigid sensors) and signal reading formats (physical vs digital systems). The emerging nano-bio interfaces have created new opportunities for developing advanced sensing technologies with unparalleled sensitivity and specificity. In this talk, I will present the development of conformal nano-bio interfaces that allow for the seamless integration of nanoelectronic interfaces into biological systems for sense digitalization with maintaining function even under deformed states. In addition, I will discuss the recent development of a biphasic, nano-dispersed (BIND) interface that can reliably connect soft, rigid, and encapsulation modules without the need for pastes. This interface was used to create stretchable devices for in vivo neuromodulation and on-skin electromyography. The modular integration improves signal quality and electrode performance, simplifying and accelerating the development of on-skin and implantable stretchable devices.

Award Lecture : **AWARD1-1**

Award Lecture - 2023 Academic Excellence Award

Room 304+305+306 FRI 13:30

Chair: Zee Hwan Kim (Seoul National University)

Pure dephasing, quantum decoherence, and wave-particle duality

Minhaeng Cho

Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science (IBS), Department of Chemistry, Korea University, Korea

Ultrafast spectroscopy is a valuable tool for monitoring the timescales of interactions between systems and their environments, resulting in pure dephasing. The superposition of ground and excited states of a molecule in a condensed phase, created by field-matter interactions, loses its coherence due to fluctuations from surrounding molecules that interact differently with the ground and excited states. Recently, quantum decoherence has become an intense area of research due to its relevance to the quantum-to-classical transition and its critical role in developing quantum technologies such as quantum computers and cryptography. Although pure dephasing and quantum decoherence result from the same process of environmental monitoring of systems through quantum entanglement between the system and its environment, they have been studied and discussed in very different contexts with seemingly disparate terminologies. In this talk, we discuss a detailed theoretical description of pure dephasing and quantum decoherence in bosonic environments coupled to a two-level system, compare them directly, and demonstrate their connections to the wave-particle duality of isolated systems and the wave-particle-entanglement triality of composite systems consisting of systems and their environments. It is believed that this interplay of quantum decoherence with wave-particle duality will be helpful for gaining a deeper understanding of ultrafast spectroscopy from a quantum mechanical perspective and the complementarity of quantum objects interacting with their surrounding environments.

Award Lecture : **AWARD2-1**

Award Lecture - 2023 Man Jung Han Academic Excellence Award

Room 401+402 WED 13:00

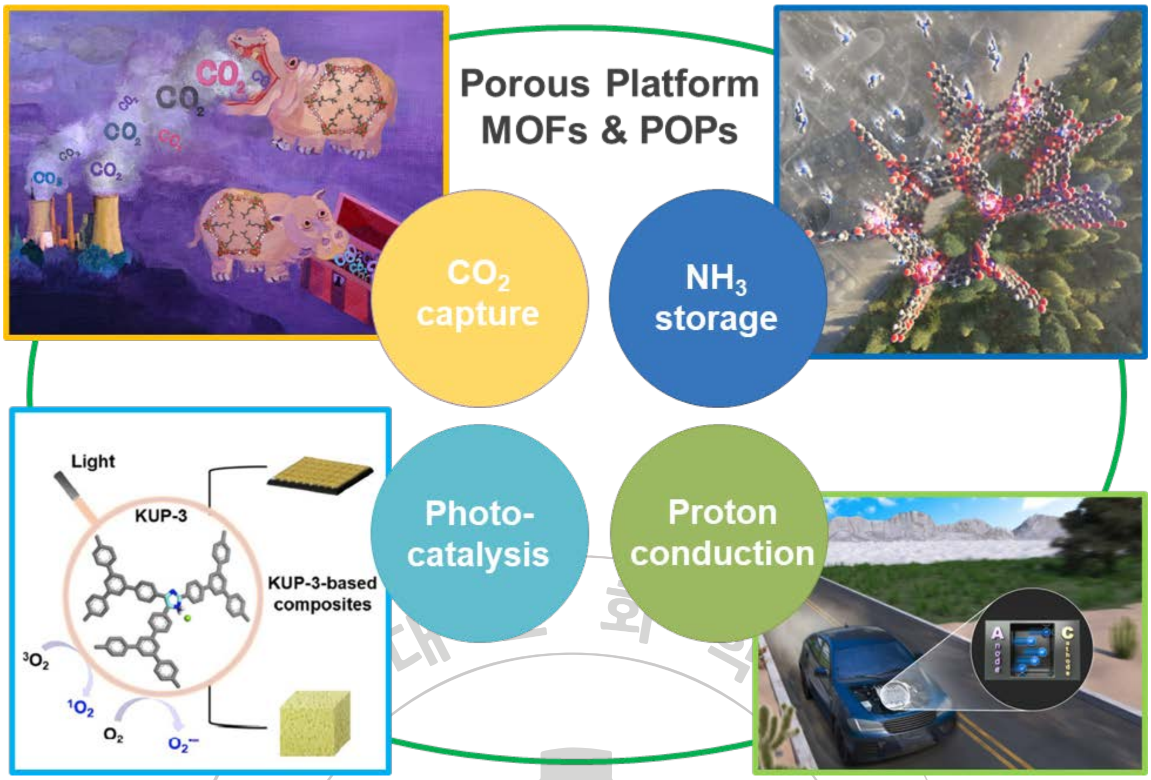
Chair: Kang Min Ok (Sogang University)

Porous Materials: Design, Post-Molecular Engineering and Desirable Properties

Chang Seop Hong

Department of Chemistry, Korea University, Korea

Porous materials such as metal-organic frameworks (MOFs) and porous-organic polymers (POPs) are emerging as porous platforms that can be used for gas adsorption and separation, sensing, catalysis, and bio applications. These solids exhibit high surface area, tunable pore size and properties, and structural diversity, making them applicable in important research fields. To imprint appropriate functionality on the platform for specific target utilization, the properties of the pore surface can be implemented through pre-design and post-molecular engineering of MOFs and POPs to endow them with optimized structural entities and improve their performance in various applications. In this talk, I will introduce the works carried out by my group on fields including gas capture, separation, conductivity, and photocatalysis using molecular design and post-synthetic modification methods of porous materials.


Porous Platform
MOFs & POPs
CO_2 capture
NH_3 storage
Photo-catalysis
Proton conduction
CO_2
Light
KUP-3
KUP-3-based composites
$^3O_2$
$^1O_2$
O_2
$O_2^{\cdot-}$
Anode
Cathode

Symposium : **KCS1-1**
[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry
Room 304+305+306 WED 13:20
Chair: So-Jung Park (Ewha Womans University)

Designed Synthesis and Assembly of Inorganic Nanomaterialsfor Energy and Catalytic Applications

Taeghwan Hyeon

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

We present a synthesis of highly durable and active fuel cell electrocatalysts based on ordered intermetallic PtM (M= Fe, Co) nanoparticles for oxygen reduction reaction.[1] We report on the design and synthesis of highly active and stable Co-N_4(O) moiety incorporated in nitrogen-doped graphene (Co_1-NG(O)) that exhibits a record-high kinetic current density and mass activity with unprecedented stability (>110 h) for electrochemical H2O2 production.[2] Guided by computation, we report a supramolecular approach for H_2O_2 electrocatalysis that uses a combination of oxygen functional groups in a carbon nanotube (CNT) substrate and a cobalt phthalocyanine (CoPc) catalyst.[3] We synthesized various multimetallic heterostructured oxide nanomaterials and investigated their structure-property relationship in energy devices and catalysis.[4] We report on the design and synthesis of highly active TiO_2 photocatalysts incorporated with site-specific single copper atoms (Cu/TiO_2) that exhibit reversible and cooperative photoactivation process, and enhancement of photocatalytic hydrogen generation and CO_2 photoreduction activity.[5] We presented a floatable photocatalytic platform constructed from elastomer-hydrogel nanocomposites, demonstrating its superiority over conventional systems in solar hydrogen production.[6]

[1] "Highly durable & active PtFe nanocatalyst for electrochemical oxygen reduction reaction," *J. Am. Chem. Soc.* **2015**, 137, 15478; "Direct Synthesis of Intermetallic Pt-Alloy Nanoparticles Highly-Loaded on Carbon Supports for Efficient Electrocatalysis," *J. Am. Chem. Soc.* **2020**, *142*, 14190; "Practical solid-state production of Pt-Co electrocatalyst for high-power proton-exchange-membrane fuel cell," *Energy Environ. Sci.* **2023**.

[2] "Atomic-level tuning of Co-N-C catalyst for high-performance electrochemical H_2O_2 production," *Nature Mater.* **2020,** *19*, 436.

[3] "Hydrogen peroxide electrosynthesis using an electronically tuned molecular electrocatalyst," *Nature Catal.* **2023**.

[4] "Design and Synthesis of Multigrain Nanocrystals via Geometric Misfit Strain," *Nature* **2020**, 359, 577; "Facet-defined strain-free spinel oxide for oxygen reduction electrocatalysis," *Nano Lett.* **2022**, *22*, 3636–3644.; "Structural Insights into Multi-Metal Spinel Oxide Nanoparticles for Boosting Oxygen Reduction Electrocatalysis," *Adv. Mater.* **2022,** *34*, 2107868.

[5] "Reversible and cooperative photoactivation of single-atom Cu/TiO_2 photocatalysts," *Nature Mater.* **2019**, 18, 620; "Electronic interaction between transition metal single-atoms and anatase TiO_2 boosts CO_2 photoreduction with H_2O," *Energy Environ. Sci.* **2022**, *15*, 601.

[6] "Floatable photocatalytic hydrogel nanocomposites for large-scale solar hydrogen production," *Nature Nanotech.* **2023**.

Symposium : **KCS1-2**

[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry

Room 304+305+306 WED 13:50

Chair: So-Jung Park (Ewha Womans University)

Next generation of nanovaccines based on membrane vesicles

Guangjun Nie

National Center for Nanoscience and Technology, China

It has witnessed that the rapid development at the interfaces of immunotherapy and nanomaterials, especially wide applications of LNP-based mRNA vaccines for COVID-19. Nanovaccines holds a great promise as a feasible and fruitful strategy, to improve the therapeutic outcomes of the current vaccines as well as fully new types vaccines for deadly diseases, such as cancers. This presentation will feature our recent development on using bacterial outer membrane vesicles (OMVs) and hybrid membranes to regulate tumor immune microenvironment to re-store the homeostasis of tumor microenvironment and/or stimulate antitumor immunity. Those systems have great potential as intelligent vehicles to enable the delivery of various potent antigens and adjuvants, which otherwise never could be used as therapeutics due to numerous limitations. Given the robust self-assembly behavior, exceptional designability, potent antitumor activity and minimal in vivo adversity, the nanovaccines represent a promising strategy for next generation of cancer therapeutics.

Symposium : **KCS1-3**

[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry

Room 304+305+306 WED 14:20

Chair: Seong-Ju Hwang (Yonsei University)

Chemistry of 2D Carbides, Nitrides, Oxycarbides, and Carbonitrides (MXenes)

Yury Gogotsi

A.J. Drexel Nanomaterials Institute, and Department of Materials Science and Engineering, Drexel University, United States

Discovery of new materials provides moments of inspiration and shifts in understanding, shaping the dynamic field of materials science. Following the discovery of 2D Ti3C2 in 2011 [1], 2D carbides, oxycarbides, carbonitrdes and nitrides of transition metals known as MXenes [2] have further expanded the nanomaterials family. More than 50 different carbide and nitride MXenes have been reported, and the structure and properties of numerous other MXenes have been predicted. Moreover, the availability of solid solutions on M and X sites, multi-element high-entropy MXenes, control of surface terminations, and the discovery of out-of-plane ordered double-M o-MXenes (e.g., Mo2TiC2), as well as in-plane ordered i-MXenes (e.g., Mo4/3C) offer a potential for producing dozens of new distinct structures and an infinite number of solid solutions. Many of those materials offer unique and very useful properties. This presentation will describe the state of the art in the manufacturing of MXenes, their delamination into single-layer 2D flakes and assembly into films, fibers and 3D structures. Synthesis-structure-properties relations of MXenes will be addressed on the example of Ti3C2. The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications.

[1] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J.-J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, Two-Dimensional Nanocrystals Produced by Exfoliation of Ti3AlC2, Advanced Materials, 23 (37), 4248-4253 (2011)

[2] A. VahidMohammadi, J. Rosen, Y. Gogotsi, The World of Two-Dimensional Carbides and Nitrides (MXenes), Science, 372, eabf1581 (2021)

Symposium : **KCS1-4**

[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry

Room 304+305+306 WED 14:50

Chair: Seong-Ju Hwang (Yonsei University)

Multiscale Nanomaterials for Chemical Sensing Applications

Il-Doo Kim

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

Electrospun nanofibers, as the forefront of advanced fibrous materials, hold extraordinary potential applications ranging from environmental, energy to biology owing to their integrated advantages of fine diameter, extremely high aspect ratio, and ease of scalable synthesis from various materials. In this talk, I summarize recent progress and a collection of advances, particularly focused on the synthesis, characterization, and utilization of electrospun polymeric membranes, highly porous metal oxide, and conducting carbon nanofibers. For multiscale integration of hetrostructured materials, tight anchoring of catalyst materials on porous supports is important. Several case studies will be discussed, especially for applications in chemical sensors with high sensitivity and selectivity. I will end my presentation by suggesting possible future research direction and potential suitability of 3D nanofibers and 1D high density yarn for applications in outstanding colorimetric sensors, exhaled breath gas analyzing sensors for early stage disease diagnosis. I will conclude my presentation by suggesting future research directions and potential suitability of the nanostructured functional nanofibers for commercial applications.

Symposium : **KCS1-5**
[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry
Room 304+305+306 WED 15:50
Chair: Hye Ryung Byon (KAIST)

Emerging nanophotonic platforms for personal and population health

Jennifer A. Dionne

Department of Materials Science and Engineering and Department of Radiology, Stanford University, United States

We present our efforts to develop photonic sensors suitable for field-deployment that enable early disease onset, help inform optimal treatment, and uncover new biological pathways associated with personal, population, and ecosystem-level health. First, we combine Raman spectroscopy and deep learning to accurately classify bacteria by both species and drug susceptibility in a single step. With a convolutional neural network (CNN), we achieve species identification and antibiotic susceptibility accuracies similar to leading mass spectrometry techniques. We show how this technique can be applied to rapid tuberculosis detection, as well as to waste-water monitoring of bacterial pathogens. Next, we describe resonant nanophotonic surfaces that enable detection of genes, proteins, and metabolites with femtomolar sensitivity. These metasurfaces produce a large amplification of the electromagnetic field intensity, increasing the response to minute refractive index changes from target binding; simultaneously, the light is beam-steered to particular detector pixels. By combining metasurface design with acoustic bioprinting for functionalization, we develop chips that detect gene fragments, proteins, and metabolites on the same platform. We discuss integration of these sensors with workflows in Stanford’s Clinical Virology Laboratory, as well as with autonomous underwater robots from Monterey Bay Aquarium Research Institute (MBARI) for real-time phytoplankton detection.

Symposium : **KCS1-6**

[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry

Room 304+305+306 WED 16:20

Chair: Hye Ryung Byon (KAIST)

Designer nanoparticles for biological targets: the case of magneto-genetics (MG)

Jinwoo Cheon

Department of Chemistry, Yonsei University, Korea

Nanochemistry has been critical for next-generation biomedical sciences with new tools that can accurately image, identify, and execute desired missions in a selectively programmed manner. In this talk, I will discuss magnetic nanoparticles as core platform materials and tools4 for a variety of functionalities such as sensing2,3,6 targeting and signaling of cells and live animals1,5 in a selective and efficient way. These tools serve as a modulator for cell signaling of neurons via magneto-genetics for the behavior control of live animals. This is a new approach of controlling neurons via magnetism which will serve for deep brain stimulations via remote and wireless fashion.

Symposium : **KCS1-9**
[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry
Room 304+305+306 WED 16:50
Chair: Yousung Jung (KAIST)

Doubly hybrid functionals: From molecules to extended materials

Xin Xu

Fudan University, China

Density functional theory (DFT) is now the most popular computational method in materials science. As the new generation functionals, doubly hybrid approximations (DHAs) have been shown to improve over conventional functionals with unprecedented accuracy in describing various kinds of chemical interactions and properties for finite molecules [1-3]. Recently, we have realized the periodic implementations of DHAs and demonstrated that the accuracy of DHAs achieved for finite molecules can be transferred to extended materials [4-7]. We anticipate that this new advancement will boost the predictive power for accurate descriptions of molecular crystals, as well as those of molecule-surface interactions in heterogeneous catalysis.

[1] Y. Zhang, X. Xu, and W.A. Goddard III, Proc. Natl. Acad. Sci. USA, 106 (2009) 4963.
[2] I. Y. Zhang, X. Xu, Y. Jung, and W.A. Goddard III, Proc. Natl. Acad. Sci. USA, 108 (2011) 19896.
[3] N. Q. Su, Z. Zhu, X. Xu, Proc. Natl. Acad. Sci. USA, 115 (2018) 2287.
[4] S. Duan, I. Y. Zhang, Z. Xie, X. Xu, J. A. Chem. Soc. 142 (2020) 6902.
[5] B. Chen, X. Xu, J. Chem. Theory Comput. 16 (2020) 4271.
[6] Y. Wang, Y. Li, J. Chen, I. Y. Zhang, X. Xu, JACS Au 1 (2021) 543.
[7] Z. Chen, Z. Liu and X. Xu, Nat. Comm. 14 (2023) 936.

Symposium : **KCS1-10**
[ACS Publications Summit at 2023 KCS Spring Meeting] Post-pandemic Transformations and Challenges in Nanoscale and Materials Chemistry
Room 304+305+306 WED 17:20
Chair: Yousung Jung (KAIST)

van der Waals layered materials: From synthesis to applications

Young Hee Lee

Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University, Korea

Since the discovery of graphene exfoliated from bulk graphite by a scotch tape, numerous unprecedented physics and chemistry phenomena including superconductivity, topological insulator, Weyl semimetal, etc. have been explored fundamentally. Yet, applications to, for example, electronics, soft electronics, optoelectronics, spintronics, and valleytronics have been hindered by the limited flake sizes of a few micrometers. Furthermore, fundamental sciences and applications are often obscured fue to the absence of single crystal film. In this talk, we will discuss some of the recent progresses on wafer-scale singlecrystal growth of 2D van der Waals layered materials including monolayer and multiplayer graphene, hBN, and transition metal dichacogenides, and their heterostructures on various substrates and further some of the applications.[1-9] This includes magnetic semiconductors by introducing dilute amount of magnetic dopants to target towards Curie room-temperature and gate tunability for spintronics and graphene/MoS2 heterostructure for next-generation solar cell via hot carriers and carrier multiplication beyond Shockley–Queisser limit.

[1] V. L. Nguyen et al., Adv. Mat. 27 (2015) 1382.
[2] V. L. Nguyen et al., Nature. Nano. 15 (2020) 861.
[3] J. S. Lee et al., Science 362 (2018) 817.
[4] S. H. Choi et al., Adv. Mat. 33 (2021) 2006601.
[5] K. Paul et al., Nat. Rev. Phys. 3 (2021), 178.
[6] T. Lan-Anh Lee et al., ACS Nano 15 (2021), 20267.
[7] T. Nguyen et al., Adv. Sci. 8 (2021), 102911.
[8] S. J. Yun et al., Adv. Mat. 34 (2022) 10.

[9] S. Choi et al., Nat. Comm. 13 (2022), 1484.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **KCS2-1**
[Tutorial 1] Writing a Scientific Paper in English
Room 401+402 WED 14:00
Chair: Tae Kyu Kim (Yonsei University)

Writing a scientific paper in English

Dongho Kim

Department of Chemistry, Yonsei University, Korea

Writing a scientific paper in English requires a set of writing skills specific to the scientific field. It is important to provide accurate and concise information. Firstly, the title should summarize the topic being written about and be clearly stated. Secondly, the introduction should explain the purpose and background of the paper in detail to give readers an appropriate expectation of the topic. Thirdly, the body should analyze the topic thoroughly using results from experiments, graphs, statistics, etc. and provide an interpretation of the main results to support the topic. Finally, the conclusion should summarize the results obtained and suggest future research plans. Precise language and structure are crucial elements in writing a scientific paper in English.

Symposium : **KCS2-2**
[Tutorial 2] Computational Chemistry: Hands-on Electronic Structure Calculations
Room 401+402 WED 16:10
Chair: Yunmi Lee (Kwangwoon University)

Computational Chemistry: Hands-on Electronic Structure Calculations

Eunji Sim

Department of Chemistry, Yonsei University, Korea

Predicting reaction dynamics and/or material properties by computational chemistry is important in modern chemistry and materials research. In particular, quantum chemistry is useful for understanding and interpreting experimental results because it enables calculation of electronic structures, including energies and geometric information that determine the physical properties and reactivity of molecules. Researchers have developed a variety of computational methods, which vary in the level of resources required and the accuracy of the results. Among them, Density Functional Theory (DFT) has been confirmed to make predictions that are in agreement with experimental observations in various fields. It is one of the most popular computational methods in recent studies due to its relatively low cost (computational time and computational resources required for computation).

This tutorial outlines the basic principles of quantum chemistry electronic structure calculations and practices basic computational procedures using various calculation methods. From writing the input file to interpreting the output file, it is a hands-on exercise for beginners without quantum computing experience.

※Participants should prepare a personal laptop with internet access and a Google Colaboratory account ready to run PySCF Python code.

Symposium : **KCS3-1**
[BKCS Symposium] Future of the Korean Chemistry
Convention Hall2 THU 15:40
Chair: Eunsung Lee (POSTECH)

Current State of the BKCS and Future Strategy

Nak Cheon Jeong

Department of Physics & Chemistry, DGIST, Korea

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

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **KCS3-2**
[BKCS Symposium] Future of the Korean Chemistry
Convention Hall2 THU 16:00
Chair: Eunsung Lee (POSTECH)

Time-Resolved Studies of Chemical Reactions: Progress, Challenges, and Future Research Directions

Hyotcherl Ihee

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

One fundamental area of Physical Chemistry is the study of chemical reactions, encompassing their mechanisms, kinetics, and thermodynamics. Time-resolved studies of chemical reactions aim to grasp the temporal evolution of chemical systems, from the initiation of a reaction to its completion. In recent years, time-resolved studies have made significant advancements, particularly in the development of cutting-edge techniques, such as femtosecond X-ray liquidography, femtosecond serial crystallography, ultrafast electron diffraction, and ultrafast electron/X-ray imaging. These methods allow for direct observation of molecular structural changes on femtosecond time scales, providing new and valuable insights into the dynamics of chemical reactions and the governing mechanisms. However, even with these advancements, challenges still persist in the field. One of these challenges is the limitations of these techniques, which are primarily confined to studying unimolecular reactions and are less effective in examining more complex or less controlled samples. Another challenge is the integration of time-resolved data with other types of information to provide a comprehensive picture of reaction dynamics. Future avenues for addressing these challenges can be explored. (Acknowledgement: This work was supported by the Institute for Basic Science (IBS-R033)).

Symposium : **KCS3-3**
[BKCS Symposium] Future of the Korean Chemistry
Convention Hall2 THU 16:25
Chair: Eunsung Lee (POSTECH)

Two-Dimensional Confined High-Pressure Nanoreactors

Hyeon Suk Shin

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

Chemical reactions conducted at high pressures provide opportunities for realising new synthesis chemistries and achieving novel states of matter. Many industrial chemical reactors operate at pressures of few thousand atmospheres but facile application of very high pressures (>1 GPa), where interesting reactions can occur and new materials can be realized, is challenging. Confinement of reactants within nanoscale spaces of low dimensional materials (pores such as zeolites and metal organic frameworks and carbon nanotubes) has been shown to provide non-equilibrium conditions for synthesis of novel molecules3 and tuning of chemical reactivity. While few studies have reported chemistry within zero dimensional pores and one dimensional nanotubes, organic reactions in confined spaces between 2D materials have yet to be explored. In this talk, I will demonstrate that reactants confined between atomically thin sheets of graphene or hexagonal boron nitride experience pressures as high as 7 GPa, which allows the propagation of solvent-free organic reactions that ordinarily do not occur under standard conditions. Specifically, we show that cyclodehydrogenation of hexaphenylbenzene without catalysts as a proof of concept and oxidative polymerisation of dopamine into sheet-like crystalline structure are enabled by the effective high pressure experienced by the reactants between the graphene layers. The graphene/polydopamine/graphene reaction results in a novel composite material that possesses higher Young’s modulus (430 GPa) than pure graphene layers (300 GPa) and an exceptionally low water vapor transmission rate of < 0.1 g-m-2-day-1 – nearly an order of magnitude lower than the state-of-the-art water-diffusion barriers for graphene and hBN. Our results demonstrate a facile, general approach for performing new high-pressure chemistry based on confinement of reactants within graphene layers that provides opportunities for realizing new materials with extraordinary properties.

Symposium : **KCS3-4**
[BKCS Symposium] Future of the Korean Chemistry
Convention Hall2 THU 16:50
Chair: Sun-Joon Min (Hanyang University)

Developing De Novo Glycochemistry Based Upon Asymmetric Metal Catalysis

Young Ho Rhee

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

Glycosides represent one of the most fundamental and highly important structural motif not only in chemistry but also in other related fields. For example, O-glycosides are found in numerous bioactive natural products and pharmaceuticals as well as oligosaccharides playing a key role in cell-cell recognition, cell growth regulation, differentiation, and immunological responses. In addition, N-glycosides play a key role in developing antiviral and anticancer pharmaceuticals. The glycosides often exist as a conjugate to complex aglycons such as polypeptides and aromatic polyketides. Despite these significances, synthetic methods towards O-/N-glycosides are very limited, due to the poor reactivity of the heteroatom nucleophiles.In this presentation, a conceptually new approach towards glycoside synthesis will be introduced. A key feature of this de novo method is represented by the glycosidic bond formation by way of the metal-catalyzed asymmetric coupling reaction of various heteroatom nucleophiles and alkoxyallene. Notably, heteratom nucleophiles, which has been considered as poor nucleophiles in classical glycochemistry, work mostly efficiently in this reaction. Thus, glycosidic bonds are formed with no activators in this reaction. Combination of this method with other chemoselective metal catalysis provides a highly efficient access to a variety of structurally complex O- and N-glycosides.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **KCS3-5**

[BKCS Symposium] Future of the Korean Chemistry

Convention Hall2 THU 17:15

Chair: Sun-Joon Min (Hanyang University)

Easier said than done: Paradigm-shifting research & disruptive innovation

Mu-Hyun Baik

Chemistry, Korea Advanced Institute of Science and Technology, Korea

The Korean Chemical Society has achieved remarkable growth and elevated chemical research in Korea to an internationally competitive level. As a consequence, there is now a heightened demand for originality, creativity, and innovation in research. It is no longer sufficient to simply produce good research; researchers must aim for paradigm-shifting breakthroughs that are disruptively innovative. Nevertheless, translating these ambitious goals into practical outcomes poses a significant challenge. In this presentation, I will share my strategies and experiences in attempting to generate the type of research that meets the public's high demand.

Symposium : **KCS4-1**
“Laboratory Safety Education for the Graduate Students and Researchers” Initiated by the Korean Chemical Society
Room 204 FRI 14:30
Chair: Ik-Mo Lee (Inha University)

Reforming the Designation and Control system for Hazardous Chemical Substance

Pong Gyun Park

National Institute of Chemical Safety, Korea

In 2023, a major shift in chemical management policy is underway in South Korea.The current chemical safety management system is based on the 'three chemical acts': the Chemical Substances Control Act, the Act on Registration and Evaluation of Chemicals (K-REACH), and the Consumer Chemical Products and Biocides Safety Control Act, which were enacted after the humidifier disaster and the Gumi hydrofluoric acid spill.The institutional framework has advanced with the enforcement of the three Acts, and accidents caused by chemicals are decreasing accordingly. By the way, industry argues that the rapid policy changes led by the government have not reflected on-site conditions, causing excessive burdens. On the other hand, civil society claims that it is difficult to feel the effects of the changed policies and that the management of high-risk substances such as environmental hormones and carcinogens is insufficient.In order to address these issues, the Ministry of Environment launched the Chemical Safety Policy Forum in 2021, in which stakeholders such as industry and civil society participate to discuss ways to overcome problems and improve the effectiveness of chemical safety system.The directions for reforming the system under discussion at the forum are: 1) Reorganization of the Designation and Control scheme, which differentiates standards by categorizing hazardous chemical substances into acute, chronic, and eco-toxicity; 2) Raising the registration threshold for chemicals under the Act on Registration and Evaluation of Chemicals and introducing a 'Korean CLP' to ensure the safe use of substances below the registration threshold; and 3) Developing a management plan for chronic toxic substances.The Ministry of Environment plans to submit draft amendments of the Chemical Substances Control Act and K-REACH to the National Assembly this year after synthesizing the discussions at the forum.In this session, Mr. Ponggyun Park, President of the National Institute of Chemical Safety will provide an overview of the revision of the chemical Acts and how these changes relate to laboratory safety.

Symposium : **KCS4-2**
“Laboratory Safety Education for the Graduate Students and Researchers” Initiated by the Korean Chemical Society
Room 204 FRI 15:30
Chair: Ik-Mo Lee (Inha University)

Three Decades of Investigating the Cardiovascular Health Effects of Chemical Exposure

Jin-Ho Chung

College of Pharmacy, Duksung Women's University, Korea

Toxicology is an essential field of study that focuses on understanding the effects of chemicals on living organisms. Over the years, significant progress has been made in this field, and toxicologists have played a critical role in identifying the harmful effects of various chemicals on human health and the environment. This lecture will provide an overview of the current state of toxicology, highlighting some of the key advancements and challenges that have shaped the field. Topics to be covered include the development of new testing methods, the identification of emerging toxins, the role of genetics in toxicity, and the importance of risk assessment in determining safe levels of exposure. The second part of talk will focus on our recent research on arsenic in drinking water, which is a worldwide health problem associated with cardiovascular disease and cancer. The speaker will discuss their research findings, which provide new insights into the mechanisms of arsenic-induced cardiovascular disease and tumor metastasis. Of a particular note, cardiovascular diseases and tumor metastasis induced by arsenic was abolished by blockers of platelet activation like aspirin, demonstrating that anti-platelet agents may be effective for preventing arsenic-associated human diseases. Overall, this lecture aims to provide a comprehensive overview of the past, present, and future of toxicology and its crucial role in protecting human and environmental health.

Award Lecture in Division : **POLY1-4**

Recent Advances in Covalent Adaptive Network Polymers

Room 303 THU 17:05

Chair: Chiyoung Park (DGIST)

Chemical Sensors and Biobased High-Performance Polymers

Byungjin Koo

Department of Polymer Science and Engineering, Dankook University, Korea

This lecture consists of two parts. First, chemical sensors based on functional aromatics and polymers are discussed. A novel lithium-sensing compound consisting of naphthalene-crown ether was synthesized via Buchwald-Hartwig amination. This compound could detect lithium ions in acetonitrile through absorption and fluorescence spectroscopy. In addition, novel amine-sensing polymers with carbon nanotubes were synthesized. The synthesis included bromination of poly(3-hexylthiophene), followed by a lithium-halogen exchange reaction and quenching with an electrophile, affording trifluoromethyl ketone-functionalized poly(3-hexylthiophene). Improved sensitivity for amine gas sensing was observed. Second, synthesis and application of biobased polymers are presented. Monomers include phenol (from lignin), butanol (from microorganism), and vanillin (from vanilla), and applying polymerization reactions such as RAFT and ROMP is presented to form biobased elastomers and pressure-sensitive adhesives (PSAs).

Symposium : **POLY1-1**
Recent Advances in Covalent Adaptive Network Polymers
Room 303 THU 15:40
Chair: Chiyoung Park (DGIST)

Photo-vitrimerization of Thermosetting Polymer

Chae Bin Kim

Department of Polymer Science and Engineering, Pusan National University, Korea

Driven by sharply growing global concerns, the demand for polymer recycling is increasing. The lack of processability of thermosets significantly limits their recycling because the simplest and most economical way to recycle polymers with the lowest carbon footprint is repairing/re-melting them into new products. Vitrimers with networked structure can relax stress and flow by triggering associative network exchanges with a maintained network density, exhibiting both thermoset and thermoplastic-like properties. However, the bond exchange chemistries for most vitrimers are thermally activated, meaning that a limited temperature range exists for vitrimers to behave as strong thermosets. From a practical perspective, a particularly useful material can be realized if it behaves as a thermoset until it needs to be recycled or repaired. To this end, in this presentation, an approach to spatiotemporally converting a thermoset to a heat-processable and self-healable vitrimer will be presented.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **POLY1-2**
Recent Advances in Covalent Adaptive Network Polymers
Room 303 THU 16:05
Chair: Chiyoung Park (DGIST)

Design of liquid crystalline epoxy resin as vitrimer by introducing covalent adaptive network

Hyeonuk Yeo

Department of Chemistry Education, Kyungpook National University, Korea

Thermosets are extensively used in a diverse range of materials ranging from daily-use substances to aerospace materials. However, unlike thermoplastic, most thermosets are insoluble and infusible after curing, which hinders their reprocessing and recycling. To solve this reuse-related issue, numerous studies have recently been conducted on thermosets that behave as thermoplastic when their crosslinked structure dissociates under certain conditions owing to their dynamic crosslinking covalent bonds. However, existing cutting-edge materials typically exhibit a trade-off relationship between their environmental friendliness and functionality. Therefore, materials such as vitrimers, which have been found to show limitations in fundamental investigations, require enhancements in their electrical, optical, and thermal properties. But, designs focused on functionalities are difficult to realize because the critical aspect in vitrimer development is the utilization of chemical groups as dynamic bonds. Here, our group has synthesized several thermosets with high thermal conductivity by exploiting the self-assembly of liquid-crystalline (LC) compounds, thus proving the effectiveness of our molecular design approach. The driving force for LC assembly is based on $\pi-\pi$ interactions, and the LC molecular design adopted in this context often involves ester and imine functional groups in conjugation with aromatic structures. Based on this approach, novel structures that could simultaneously form mesogenic structures and covalent adaptive network were designed. In the presentation, the details of molecular design, synthesis, characterization and properties will be discussed.

Symposium : **POLY1-3**
Recent Advances in Covalent Adaptive Network Polymers
Room 303 THU 16:40
Chair: Chiyoung Park (DGIST)

Supramolecular chemistry in polymer network

Jiheong Kang

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

Dynamically crosslinked polymeric materials have found widespread applications in a sustainable society. However, coherent strategies for mechanically tough dynamic polymers are still lacking due to a trade-off relationship between mechanical robustness and viscoelasticity. Recently, our group used supramolecular assembly as a tool box for the design of mechanically tough dynamic polymers. We have extensively studied the effects of supramolecular stickers and their multi-scale assembly on the dynamic mechanical behaviors of polymer networks. In my presentation, I will discuss the details of their structure and functions. Their new applications will be introduced as well

Symposium : **POLY2-1**
Special Symposium by Mid-career Polymer Chemists
Room 303 FRI 09:00
Chair: Changsik Song (Sungkyunkwan University)

Nitric oxide modulation for the treatment of inflammatory diseases

Won jong Kim

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

Nitric oxide (NO) plays various physiologically favorable roles in the body. However, excessive production of NO causes inflammation and leads to various chronic inflammatory diseases. A typical NO-related disease is rheumatoid arthritis (RA), and it is well known that NO is a critical molecule for inflammation in the pathophysiology of RA. Therefore, depletion of NO can be an attractive treatment option for RA. In this study, we are reporting several strategies for the treatment of inflammatory disease via removing NO in disease site. In special, we designed an injectable in situ polymeric aggregate-embodied hybrid NO-scavenging and sequential drug-releasing (M-NO) gel platform for the combinatorial treatment of RA by incorporating a “clickable” NO-cleavable cross-linker (DA-NOCCL). This network is held together with polymeric aggregates to achieve a self-healing capability for visco-supplementation and on-demand dual drug (both hydrophilic and hydrophobic)-releasing properties, depending on the NO concentration. Moreover, consecutive NO-scavenging action reduces pro-inflammatory cytokine levels in LPS-stimulated macrophage cell lines in vitro. Finally, the intra-articularly injected M-NO gel with anti-inflammatory dexamethasone significantly alleviated the symptoms of RA, with negligible toxicity, in animal models. We believe that this novel M-NO gel platform will provide a guideline for the combinatorial treatment of RA and various NO-related diseases.

Symposium : **POLY2-2**

Special Symposium by Mid-career Polymer Chemists

Room 303 FRI 09:25

Chair: Changsik Song (Sungkyunkwan University)

The use of mutiscale responseive hydrogel for biosensor and soft actuator

Won-Gun Koh

Yonsei University, Korea

We present two different application of multiscale responsive hydrogel, which can be prepared by electrospinning or micropatterning processes. The first application is the use of bioresponsive hydrogel for biosensing. we monitored the volume changes of bioresponsive hydrogels using the concept of moiré patterns. To generate a moiré pattern, a hydrogel grating with microgroove patterns was fabricated via replica molding, which was then overlaid with a reference grating with a different pitch size. Although the change in the pitch size of the hydrogel grating due to external stimuli was small, a much greater signal could be obtained when moiré signals were used. After the pH-responsiveness of the hydrogel was successfully monitored using a moiré pattern, quantitative detection of the target protein was performed using an antibody-incorporated hydrogel. The second application is the use of responsive hydrogel for soft actuators. We fabricated a soft actuating system based on hydrogel-incorporated fibers by combining electrospinning and hydrogel lithography. Fibrous passive and active layers were stacked and connected together by a hydrogel micropattern coupling layer. The combination of stimuli-responsive PAA or PNIPAAm with a PCL-based passive layer caused the bending and unbending of the multilayered fibrous actuator when the pH or temperature was changed. The computational simulation was also performed and revealed that the bending characteristics of the actuator are determined by the size and mechanical properties of the active layer relative to those of the coupling layer.

Symposium : **POLY2-3**
Special Symposium by Mid-career Polymer Chemists
Room 303 FRI 10:00
Chair: Changsik Song (Sungkyunkwan University)

Lipid Nanoparticle Technology for RNA delivery

Eun-Kyoung Bang

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

There are various materials used to improve the stability and delivery of RNA therapeutics, but among them, lipid nanoparticles (LNPs) have already been approved as new siRNA formulations (Onpattro®, Alnylam) in 2018 and have rapidly being applied to the COVID-19 mRNA vaccine as well. The LNP formulations of currently approved mRNA vaccines are not significantly different from Onpattro®, and both of these delivery technologies are based on the same patent. Based on our experience in siRNA delivery technologies using various methods such as direct modification, conjugation, cationic lipids, and cationic polymers, we are currently working on LNP-based delivery for RNA therapeutics.The composition of LNPs has been variously reported to include ionic lipids, phospholipids, cholesterol and PEG-conjugated lipids. Among them, helper lipids and cholesterol account for about 30 to 50% of the total as structural lipids to maintain the skeleton of LNP, and it is said that 30 to 40% of the LNP formulation should be maintained with the structural lipids. PEG-conjugated lipids are used to determine size and ensure particle stability by preventing aggregation between particles. PEG is found in many medications that sometimes cause anaphylaxis. Some allergists and immunologists believe that "a minority of people who have already been exposed to PEG have high levels of antibodies to PEG, putting them at high risk of developing an anaphylactic reaction to the LNP", which is why polymers to replace PEG are being considered. In this lecture, I would like to learn about LNPs used in mRNA vaccines and briefly introduce current research.

Symposium : **POLY2-4**

Special Symposium by Mid-career Polymer Chemists

Room 303 FRI 10:25

Chair: Changsik Song (Sungkyunkwan University)

Polar Helical Columnar Assemblies

Byoung-Ki Cho

Department of Chemistry, Dankook University, Korea

Polar columnar assemblies of aromatic groups are an interesting research topic because their electric and photophysical functions can be engineered in response to electric fields. Recently, we have studied polar columnar organic materials driven by helical assembly based on 1,2,3-triazole, amide, and 1,3,4-oxadiazole groups with large dipole moments. The columnar materials organized diverse polar helical assemblies which showed interesting orientation and material properties, e.g., piezo-, ferroelectricity, tunable alignments, and polymorphism. The details regarding these issues will be addressed in the presentation.

Symposium : **POLY3-1**
Recent Trends in Polymer Chemistry for Energy Conversion
Room 303 FRI 14:30
Chair: Do Hoon Hwang (Pusan National University)

p-Type and n-type organic semiconducting materials for organic solar cells

Han Young Woo

Department of Chemistry, Korea University, Korea

Over the past few decades, organic solar cells (OSCs) have made a significant progress, showing their great potential for low-cost, flexible, lightweight, portable and large-area energy-harvesting devices. In recent years, nonfullerene acceptors have emerged as an alternative candidate of n-type materials to overcome the difficulties of fullerene derivatives in tuning optical and electronic properties. The strong and easily adjustable absorption characteristics of nonfullerene acceptors have been considered as a strong point compared to fullerene-type structures, showing a photovoltaic efficiency over ~20%. To further optimize the OSCs for next generation green energy sources, several important points need to be considered carefully. Here we discuss the fundamental correlations between molecular structure, blend morphology and device performance in fullerene- and nonfullerene acceptor-based OSCs.

Symposium : **POLY3-2**

Recent Trends in Polymer Chemistry for Energy Conversion

Room 303 FRI 14:55

Chair: Do Hoon Hwang (Pusan National University)

Ultrahigh-Quality pi-Conjugated Polymers for Organic Solar Cells

Changduk Yang

Ulsan National Institute of Science and Technology, Korea

With a growing interest in developing high-performance pi-conjugated polymers, new synthetic approaches that result in the higher-quality pi-conjugated polymers are need to help make organic optoelectronic and photovoltaic applications more prosperous. Herein, we report various methodologies for this purpose. The results discovered in this presentation should facilitate the continuous development of high-quality organic photovoltaic and organic electronic polymers.

Symposium : **POLY3-3**

Recent Trends in Polymer Chemistry for Energy Conversion

Room 303 FRI 15:30

Chair: Han Young Woo (Korea University)

Conjugate Polymers to Achieve Stability and Non-halogen Solvent Application in Organic Solar Cells

Won Suk Shin

Center for Energy Materials Metrology, Korea Research Institute of Chemical Technology, Korea

Organic solar cells (OSCs) are attracting attention due to thier colorful, transparant, flexible, and affordable mass-producible capabilities. As the efficiency of OSC is recently approaching 20%, expectations for commercialization are rising. However, commercialization standpoint, it is crucial to maintain stable efficiency in the long term, rather than initial efficiency, and to manufacture OSCs using a non-halogen solvent that can be used for production. In this presentation, it will be presented the development of photoactive polymer materials that can be processed using non-halogen solvents while also improve the stability of organic solar cells.

Symposium : **POLY3-4**

Recent Trends in Polymer Chemistry for Energy Conversion

Room 303 FRI 15:55

Chair: Han Young Woo (Korea University)

Stretchable and Thermally Stable Polymer Ionic Conductors for Energy Devices

Taiho Park

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

Stretchable electronics have received immense interests for the applications in biocompatible, wearable, and conformable devices. In these applications, stretchable conductors with intrinsic adhesion, toughness, and mechanical compliances play a critical role to facilitate the device constructions, in place of the commonly used materials such as metallic thin films (gold (Au), silver (Ag), and copper (Cu)). Intrinsic opacity leads to limitation for transparent applications; and solution process, which is favorable for low cost, mass production, and bioresorbability is impossible because of the solubility of the conducting materials in common organic solvents. To challenge the paradigm, ionic conductors, which can be sorted into organogels and hydrogels are developed, could partially circumvent limitations in transparency and solution processability. In this talk, I will discuss some issues related to polymer ionic conductors.

Symposium : **INOR1-1**

Bioinorganic Chemistry 101

Room 407+408 THU 15:40

Chair: Seung Jae Lee (Jeonbuk National University)

Photocatalytic Conversion of CO2 to Formate by Ni(II) Complexes and Well-organized Immobilization of Photocatalysts and Enzymes

Jinheung Kim

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

The efficient and specific photoconversion of carbon dioxide to formate is a scientific challenge especially for utilizing visible light energy and metal complexes. Two Ni(II) complexes of pyridylbenzimidazole and pyridylbenzothiazole were examined for CO2 conversion using eosin Y as a photosensitizer. The photoreaction of CO2 catalyzed by Ni complexes selectively affords formate with a high efficiency (14000 turnover number) and a high catalytic selectivity. Undesirable proton reduction pathways were completely suppressed in the photocatalytic reactions with these sulfur-rich Ni catalysts under CO2. Hydrogen photoproduction was also studied under argon. These bioinspired Ni(II) catalysts with N/S ligation in relation to hydrogenases are the first examples of early transition metal complexes affording such high selectivity and efficiencies for artificial photosynthesis. On the other hand, bioinspired photosynthetic systems composed of photocatalysts and enzymes are a notable framework for converting CO2 to high value chemicals. In this study, DNA nanosheets (NSs) were utilized as a support for selective immobilization of a Rh complex and formate dehydrogenase (FDH) for concerted catalytic reactions for CO2 reduction. Based on the face-selectivity, DNA-conjugated Rh complex and FDH were immobilized on NSs. The catalytic system exhibited CO2 conversion efficiencies highly dependent on the spatial organization of Rh complex and FDH. The photocatalyst-NS system coupled with free FDH showed 1,360 TON for the formate production based on NAD+, which is the highest value reported thus far for Rh-based photocatalyst/enzyme coupled systems. The results demonstrate that the compartmentalization of photocatalysts and biological enzymes is a viable approach for improving the efficiency of CO2 conversion and provide important design rules for building efficient artificial photosynthetic systems.

Symposium : **INOR1-2**

Bioinorganic Chemistry 101

Room 407+408 THU 16:05

Chair: Seung Jae Lee (Jeonbuk National University)

Surface and Interface Engineering in Photocatalysis for CO2 reduction

Ho-Jin Son

Department of Advanced Materials Chemistry, Korea University, Korea

We have studied a multicomponent inorganometallic (MIOM) photocatalytic system for CO2 reduction and established its working mechanism in depth, henceforth upgrading its catalytic performance including lifetime. Within this context, TiO2-mediated MIOM system was the most reliable inorganic foundation, and, therefore, much effort has been exerted on engaging molecular visible photosensitizers as well as catalysts onto the platform. The basic process of photocatalysis is initiated by the visible-light absorption by organic/organometallic dyes, followed by the charge separation and interfacial electron transfer (ET) toward catalytic center occurring on the TiO2 semiconductor surface. Since these reactions primarily occur at the interface between molecular functional components (diverse types of organic/organometallic photosensitizers and molecular Re(I)/Mn(I)/Ru(II) reduction catalysts) and inorganic solid semiconductor (mainly well-defined n-type TiO2), the ET efficiency between key components significantly affects the overall photochemical reaction kinetics and mechanism. Therefore, a proper elucidation of interfacial ET kinetics of functional components on TiO2 surface is essential to obtain the desired reactions with high efficiency. Herein, we report the details of the interfacial ET process between components and discuss the structure-activity relationships based on the relative excited-state energy levels of components. Figures below show schematic representations of possible MIOM systems related to the present investigation on the photocatalytic CO2 reduction.

Symposium : **INOR1-3**

Bioinorganic Chemistry 101

Room 407+408 THU 16:25

Chair: Seung Jae Lee (Jeonbuk National University)

A Potent Strategy for Cancer Treatment: Regulation of 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 : **INOR1-4**
Bioinorganic Chemistry 101
Room 407+408 THU 16:45
Chair: Seung Jae Lee (Jeonbuk National University)

Applications of Advanced EPR Spectroscopy in Bioinorganic Chemistry

Sun Hee Kim

Western Seoul Center, Korea Basic Science Institute, Korea

Bioinorganic chemistry is at the interface between chemistry and biology as metal ions play significant roles in biological systems. In this point of view, to conceptualize the functional roles of metal cofactors, identification of structures of active sites is essential. As Bioinorganic Chemistry 101 symposium aims to introduce fundamentals and applications of bioinorganic chemistry, my presentation will be focused on the basics and applications of characterizing metal cofactors in bioinorganic systems by using magnetic resonance spectroscopy. In particular, Electron Paramagnetic Resonance (EPR) spectroscopy, the electron spin version of magnetic resonance spectroscopy, has been proven to be a key player in the field of bio-inorganic chemistry. Our group utilizes advanced EPR spectroscopy (i.e. multi-frequency, multi-technique pulse EPR) to elucidate molecular mechanisms of bio-catalysts by placing an emphasis on revealing structures of intermediates of interesting catalytic reactions as seen in nature. In this talk, I will introduce the basic concepts and techniques of EPR spectroscopy and present examples of application of advanced EPR spectroscopy in bioinorganic chemistry with the recent results from our group.Advanced EPR spectroscopy provides accurate spin Hamiltonian values which can be used for in-depth analysis to explain the electronic structures of short-lived intermediates species during the biocatalytic reactions, hence may deepen the knowledge for understanding working mechanisms of the interesting reactions in bioinorganic chemistry.

Symposium : **INOR1-5**

Bioinorganic Chemistry 101

Room 407+408 THU 17:05

Chair: Seung Jae Lee (Jeonbuk National University)

Efficient Nicotinamide Adenine Dinucleotide Regeneration with Rhodium Catalysts and their mechanism

Sungho Yoon

Department of Chemistry, Chung-Ang University, Korea

The synthesized ligated rhodium complexes [(η5-Cp*)Rh(L)Cl]+ [Cp* = pentamethylcyclopentadienyl; L = ligand] acts as the exceptional catalyst in the reduction of NAD+ to NADH with an excellent turnover frequency compared to that of the higher catalytic activity of the commercially available catalyst [Cp*Rh(bpy)Cl]+ (bpy = 2,2'-bipyridine). Offsetting the contentious atmosphere currently taking place over the specific intermediate of the NADH regeneration, this study presents pivotal evidence of a metal hydride intermediate: a stable form of the rhodium hydride intermediate was isolated and fully characterized. This enables thorough insight into the possible mechanism and exact intermediate structure in the NAD+ reduction process.This study has important implications for the field of enzymatic transformations, as the regeneration of NADH is essential for many biological and synthetic processes. The development of highly active and stable catalysts for this process, as demonstrated in this study, can enable more efficient and cost-effective enzymatic transformations.

Symposium : **INOR2-1**

Recent Advances in Coordination Chemistry

Room 407+408 FRI 09:00

Chair: In-Hyeok Park (Chungnam National University)

Activation of Dihydrogen and Carbon Dioxide at a Cobalt Center Supported by Rigidified PNP Pincer Ligand

Jonghoon Choi

Department of Chemistry Education, Chonnam National University, Korea

Cobalt has been receiving much attention due to its versatile use as a catalyst in hydrogen evolution reaction, electrocatalysis and organic/inorganic chemical catalysis. Due to the character of cobalt such as its abundance, unprecedented reactivity and potential efficient catalysis orientating from the low activation barrier, chemists have been attracted and cobalt has been explored to inorganic/organic conversion. In particular, cobalt has been employed in the catalytic (de)hydrogenation and hydrogen evolution reaction using well-defined cobalt complexes, however, the detailed mechanism of their catalytic reactions remains unveiled. Here, syntheses and characterization of cobalt complexes supported by an acridane adapted ^{acri}PNP ligand (^{acri}PNP^{-} = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridine-10-ide) will be presented. A monovalent cobalt complex was exploited from the chemical reduction of corresponding cobalt(II) bromide species and a low spin three-coordinate cobalt complex, (^{acri}PNP)Co, was prepared from applying vacuum. Upon addition of dihydrogn, a divalent cobalt monohydride species was generated via a homolytic cleavage of H_2. The resulting cobalt-hydride species was used as a catalyst in the catalytic CO_2 hydrogenation. Further investigation on the transformation of dihydrogen and carbon dioxide will be discussed in detail.

Symposium : **INOR2-2**

Recent Advances in Coordination Chemistry

Room 407+408 FRI 09:20

Chair: In-Hyeok Park (Chungnam National University)

Photoswitching Effect in Pd(II) Cages

Haeri Lee

Department of Chemistry, Hannam University, Korea

Coordination cages act as a powerful tool for studying the confined effect. The control of structures and functions of coordination compounds by external stimuli has been a key strategy for the stabilization of reactants, catalysis, and drug delivery systems. Among various stimuli (e.g. pH, temperature, electrochemical or chemical input), light-triggered supramolecular systems have many advantages: less production of chemical waste, a rapid process, and a high degree of photoconversion. Recently, the Clever group has studied on chirality induction of coordination cages consisting of dithienylethene (DTE) link. Nevertheless, the development of light-responsive supramolecules has proven to be a highly challenging topic. Hereby, we present Pd2L4 coordination cages based on a diazocine moiety which is bridged azobenzene. Unlike azobenzene, cis-diazocine is a stable form and isomerized to trans-form under UV irradiation. The isomerization of diazocine drives significant dimensional changes in the molecular structures, as well as size-selective guest encapsulation in the cavity of cages.

Symposium : **INOR2-3**

Recent Advances in Coordination Chemistry

Room 407+408 FRI 09:40

Chair: In-Hyeok Park (Chungnam National University)

Nanoscale structural control and synergistic effects with metal–organic frameworks

Juyeong Kim

Department of Chemistry, Gyeongsang National University, Korea

Hybrid nanostructures, combined with a metal nanoparticle core and a porous inorganic shell, have shown new functions and properties in sensing, catalysis and adsorption, which cannot be achieved from their single component. Although various combinations between core and shell materials such as activated carbon, mesoporous silica and zeolite have been explored, further effort and time will be required to explore nanoscale structural control and synergistic effects with metal–organic framework shells. We demonstrate nanoscale control in surface modification of anisotropic gold nanoparticles with zeolitic imidazolate frameworks, and their new properties and functions are explored in surface-enhanced Raman sensing. Template-confined core transformation can also be controlled through core etching and regrowth processes, and such core transformation mechanism is understood via quantitative analysis on the core geometry and curvature. Our study will aid in the facile design and application of metal–organic framework-based hybrid materials.

Symposium : **INOR2-4**
Recent Advances in Coordination Chemistry
Room 407+408 FRI 10:00
Chair: In-Hyeok Park (Chungnam National University)

Rational Design of MOF@MOF Architectures: Synthesis, Characterization & Application

Hoi Ri Moon

Department of Chemistry and Nanosciecne, Ewha Womans University, Korea

Rational and creative design of organic and metal building blocks has successfully enabled the genesis of a variety of MOFs that are of fundamental scientific importance as well as provide a myriad of practical applications. Recently, we are aiming at the future of MOFs beyond the current limit of MOFs. In order to achieve the new function of materials, we are intensively studying the single crystalline MOF-on-MOF architectures, which are expected to show the synergistic effects that are not obtained in the original architectures. To combine the pairs of MOFs, we carefully consider the crystal structures of each MOF and the interface between them. In general, MOFs are viewed as attractive candidates to construct new composite materials given their facile synthesis and a large library of synthesized MOFs (over 70,000) that can be used as building blocks. In this talk, we present a joint computational/experimental workflow that screens thousands of metal-organic frameworks (MOFs) and identifies the optimal MOF pairs that can seamlessly “connect” to one another by taking advantage of the fact that the metal nodes of one MOF can form coordination bonds with the linkers of the second MOF. In addition, we report the composites of dimensionally (2D and 3D) and functionally (conductive and porous) different two MOFs in the form of a well-integrated core-shell structure. The hierarchically assembled 2D-MOF@3D-MOF exhibits new interfacial properties that are responsible for synergistically enhanced sensing performances toward toxic H^2S gas with the lowest recorded limit of detection (1.4 ppb), superior sensitivity ($\Delta R/R^0 = 3.36$), and outstanding selectivity at room temperature in air.

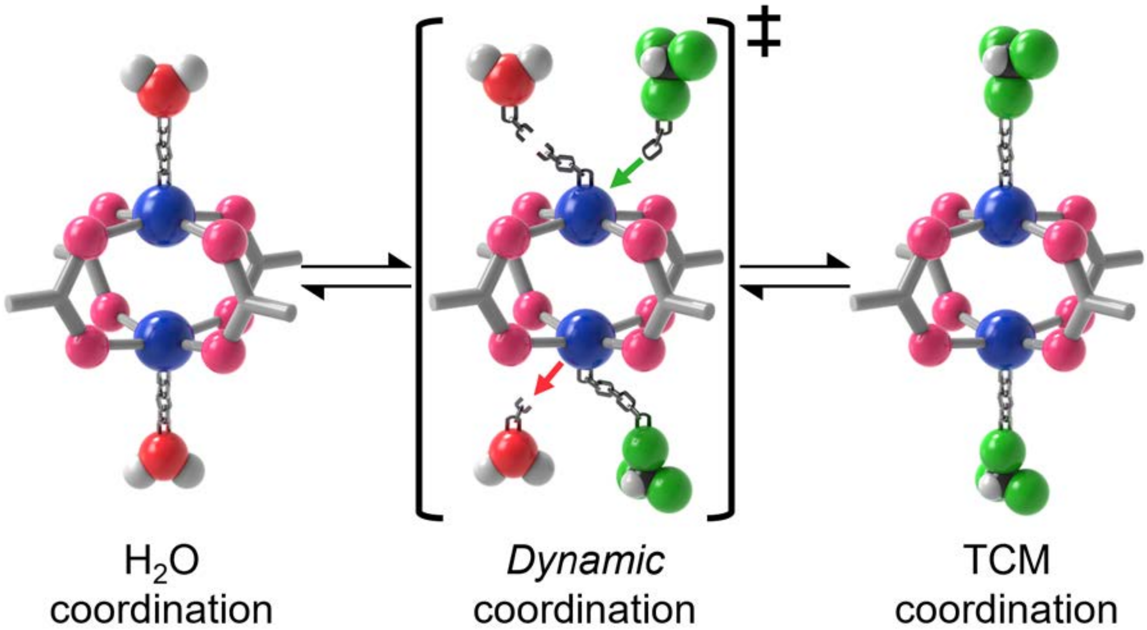
Symposium : **INOR2-5**
Recent Advances in Coordination Chemistry
Room 407+408 FRI 10:30
Chair: In-Hyeok Park (Chungnam National University)

Solvent Coordination Strength: An Essential Factor for Metal Catalytic Reactions

Nak Cheon Jeong

Department of Physics & Chemistry, DGIST, Korea

Open metal sites in metal-organic frameworks (MOFs), typically occupied by the coordination bonding of Lewis-base solvent molecules used in MOF synthesis, often play a crucial role in various catalytic reactions. In this talk, we introduce the ability of chloromethanes to form weak coordination bonding, which can provide the activation state to metal centers for catalytic reactions. More concretely, while the possible metal coordination of chloromethanes (dichloromethane and trichloromethane) has rarely been known, we show that the neutral chlorine atom in such chloromethanes can have a weak coordination bonding at metal centers, and this weak coordination can exchange relatively stronger coordination of Lewis-base molecules such as water, methanol, ethanol, and other catalytic substrates. Exploiting this weak coordination bonding, we demonstrate that the coordination exchangeability of the weak coordination bonding makes the metal center continuously activated, and thus, it substantially enhances the catalytic activity of the metal centers.


‡
H_2O coordination
Dynamic coordination
TCM coordination

Symposium : **INOR3-1**

Recent Trends in Inorganic Catalysis and Reactions

Room 407+408 FRI 14:30

Chair: Changho Yoo (KRICT)

Cu(triNHC)-catalyzed reactions converting sustainable resources to useful chemicals

Hye-Young Jang

Department of Chemistry, Ajou University, Korea

Copper complexes coordinated with tri-N-heterocyclic carbene (triNHC) were employed for sustainable catalysis; the synthesis of organic carbonates/carbamates from CO2 and the synthesis of ultralow-branched polyglycerol. A key feature of both reactions is the dissociation of one of NHC ligands from the copper ion, rendering the initial deprotonation of alcohols by the basic NHC unit. Subsequent nucleophilic addition of alkoxides completed the desired product formation. In addition, the presence of remaining bidentate NHC ligands on the copper ion increased the reactivity and stability, resulting in highly enhanced catalytic activity. In this presentation, we will demonstrate the utilization of unique Cu(triNHC) catalysts for environmentally benign catalytic processes converting renewable carbon resources.

Symposium : **INOR3-2**
Recent Trends in Inorganic Catalysis and Reactions
Room 407+408 FRI 14:50
Chair: Changho Yoo (KRICT)

Well-defined nanoplate DMC Catalysts for Propylene Oxide Homo and CO2-Copolymerizations

Bun Yeoul Lee

Department of Molecular Science and Technology, Ajou University, Korea

DMC catalyst is typically prepared by mixing K3Co(CN)6 and huge excess ZnCl2 in water to precipitate solids which should be tediously washed several times. Structure and working mechanism are still elusive and veiled. We were able to obtain well-defined DMC catalyst by reacting H3Co(CN)6 and equivalent amount of ZnCl2 in organic solvent. Given the well-defined DMC catalyst, the structure was unambiguously determined, enabling to understand the working mechanism and, eventually, to find efficient catalyst for CO2/epoxide copolymerization.

Symposium : **INOR3-3**

Recent Trends in Inorganic Catalysis and Reactions

Room 407+408 FRI 15:10

Chair: Changho Yoo (KRICT)

Cobalt(II), Copper(II) and Zinc(II) Complexes Supported by 4-(quinolin-2-ylmethyl)morpholine for Highly Stereoselective Ring-Opening Polymerization of rac-Lactide

Hyosun Lee

Department of Chemistry, Kyungpook National University, Korea

Cobalt(II), copper(II) and zinc(II) complexes supported by ligand 4-(quinolin-2-ylmethyl)morpholine (L_{QM}) have been synthesized. Structural characterization revealed distorted tetrahedral geometry around zinc(II) and cobalt(II) centers; whereas in-between distorted square planar and tetrahedral geometry has been observed for copper(II) complex. The reactivities of an in situ generated catalytic species, whereby the dichloro M(II) complexes were pre-treated with either LiMe or LiO^iPr so as to form the metal-alkyl and metal-isopropoxide derivatives, towards ROP (Ring-Opening Polymerization) of rac-lactide are studied. The catalytic system $[L_{QM}MCl_2]/LiO^iPr$ and $[L_{QM}MCl_2]/LiMe$ (M = Co, Cu, Zn) resulted in over 95% conversion within 30 seconds. The effect of an initiating group and the geometry of the metal complexes steered the heterotactic enchainment of the resultant PLA. Among the studied complexes, the $[L_{QM}CoCl_2]/LiMe$ system represents the first-ever example of ROP cobalt(II)-catalyst for rac-lactide with high heterotactic enchainment (Pr = 0.90) with 98% conversion within 5 minutes. Variations of M_n values with increasing conversion is indicative of living polymerization with $[L_{QM}MCl_2]/LiO^iPr$ and $[L_{QM}MCl_2]/LiMe$ (M = Co, Cu, Zn) systems.

Symposium : **INOR3-4**
Recent Trends in Inorganic Catalysis and Reactions
Room 407+408 FRI 15:30
Chair: Changho Yoo (KRICT)

Synthetic biomimetic inorganic compounds with DFT: some examples

Kyung-Bin Cho

Department of Chemistry, Jeonbuk National University, Korea

Our laboratory specializes in density functional theory calculations on biomimetic inorganic compounds, mimicking enzyme reactions occurring in the nature. The simplification of enzymes into small synthetic model complexes enables us to understand the core reactions occurring in the active site of enzymes without having to consider the complications that may occur due to the interference of peripheral enzyme parts. Of special interest is metal-oxygen catalyzed reactions of organic substrates, such as C-H activation, hydroxylation or other oxygen addition reactions. This presentation will mainly focus on two recent examples from our lab in collaboration with experimental groups: NO_2 conversion to RNO by a Ni(I) catalyst and aromatic deformylation by a Co(III)OOH catalyst.

Symposium : **INOR3-5**
Recent Trends in Inorganic Catalysis and Reactions
Room 407+408 FRI 15:50
Chair: Changho Yoo (KRICT)

Palladium-Catalyzed Olefin Hydrofunctionalization with Nucleophiles Enabled by Electrochemical Oxidation

Kwangmin Shin

Department of Chemistry, Sungkyunkwan University, Korea

Alkenes and other unsaturated compounds have been regarded as attractive starting materials in modern organic syntheses owing to the abundance, readily availability, and synthetic versatility of these substrates. Among the transformation of these unsaturated compounds, hydrofunctionalization, an addition of a hydrogen and a functional group across a carbon-carbon double bond, is arguably one of the most efficient methods to prepare more complex molecules from simple olefinic compounds. As a result, a diversity of approaches has been developed. Among these strategies, metal-hydride catalyzed olefin hydrofunctionalization has been received particular attention owing to the fact that the desired transformations can be achieved by suitable choice of catalyst/ligand system. Despite the great achievements, however, the majority of the developed synthetic protocols rely on the use of electrophilic coupling partners that require pre-functionalization.Here, I present our group’s research effort toward the establishment of electrocatalytic approach, in more detail, the merger of palladium catalysis with electrooxidation, for the hydrofunctionalization of olefins with nucleophiles. The first part of this talk will discuss the development of palladium-catalyzed electrooxidative hydrofluorination of olefins with nucleophilic fluorine source. In the second part, our endeavor to develop palladaelectrocatalysis for (enantioselective) hydroalkoxylation of olefins with alcohols will be discussed.

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

Recent Trends in Spectroscopy and Microscopy

Room 401+402 THU 15:40

Chair: JunWoo Kim (Chungbuk National University)

Extending density functional calculations beyond pure water

Eunji Sim

Department of Chemistry, Yonsei University, Korea

Density-corrected density functional theory (DC-DFT) reduces density-driven energy errors caused by errors in self-consistent densities by using a more accurate density instead.[1] This presentation reviews recent progress in functional design and applications based on DC-DFT, including functional error analysis utilizing density insensitive systems.[2] In particular, the systematic application of the DC-DFT principles combined with dispersion correction was used to design the HF-r2SCAN-DC4 functional, which excellently captures interactions between water molecules as well as important noncovalent interactions between water and bio- and organic molecules.[3]

[1] M.-C. Kim, E. Sim, and K. Burke "Understanding and Reducing Errors in Density Functional Calculations", Phys. Rev. Lett. 111, 073003 (2013)

[2] E. Sim, S. Song, S. Vuckovic, and K. Burke, "Improving Results by Improving Densities: Density-Corrected Density Functional Theory," J. Am. Chem. Soc., 144, 6625 (2022).

[3] S. Song, S. Vuckovic, Y. Kim, E. Sim, and K. Burke, "Extending density functional theory with near chemical accuracy beyond pure water," Nat. Commun. 14, 799 (2023).

Symposium : **PHYS1-2**

Recent Trends in Spectroscopy and Microscopy

Room 401+402 THU 16:10

Chair: JunWoo Kim (Chungbuk National University)

Molecular Cluster Spectroscopy: Correlating Structure and Chemical Reactivity

Schultz Thomas

Chemistry, Ulsan National Institute of Science and Technology, Korea

Photochemical reactivity may reflect inherent properties of the light-absorbing chromophores or may be controlled by intermolecular interactions within a local environment. Gas phase spectroscopy gives detailed insight into molecular structure and properties, but does not allow to study the effect of the local environment. Condensed phase investigations always involve a local environment, but this environment is typically heterogeneous and it is hard to identify whether particular local structures provide relevant driving forces for chemical reactions. Spectroscopy of molecular clusters in the gas phase provides a bridge between the two domains and allows to study processed in a well-defined environment. Even simple gas phase clusters show heterogeneity in terms of cluster size and cluster structure. With mass-correlated rotational alignment spectroscopy (CRASY), we developed a method to resolve this heterogeneity: the structure of neutral molecules or clusters (educt of a chemical reaction) is characterized through high-resolution rotational Raman spectra. Photochemically triggered fragmentation reactions in excited or ionized states are then observed in a mass spectrometer and can be assigned to a well-characterized cluster species. Here, we present the first successful cluster-CRASY experiment for carbon disulfide clusters. Fig. 1 shows a mass spectrum and a correlated rotational spectrum for the mass channel of the CS2 monomer. The presence of dimer rotational bands at the monomer mass reveals the presence of cluster fragmentation. A systematic correlation analysis reveals the complete parent-fragment correlation map for 22 chemical species in the mass spectrum. Surprisingly, dimer rotational bands were correlated to the SCCS and S2 cation mass channels, but not to C, S, and CS mass channels. To identify the origin of the unexpected dimer fragments, we explored the cationic potential energy surface using dispersion-corrected DFT. The minimum-energy pathway for formation of SCCS and S2 cations proceeds via two energetic transition states and a spiro-intermediate. These energetic fragments can only be formed after above-threshold ionization, explaining the small amplitude of corresponding signals.The mass-correlated rotational spectrum of the dimer (FWHM resolution of 36 MHz) also allowed us to characterized the geometry of the cluster at high resolution. The spectroscopically observed bond length and C2v symmetry agree well with theoretical predictions.

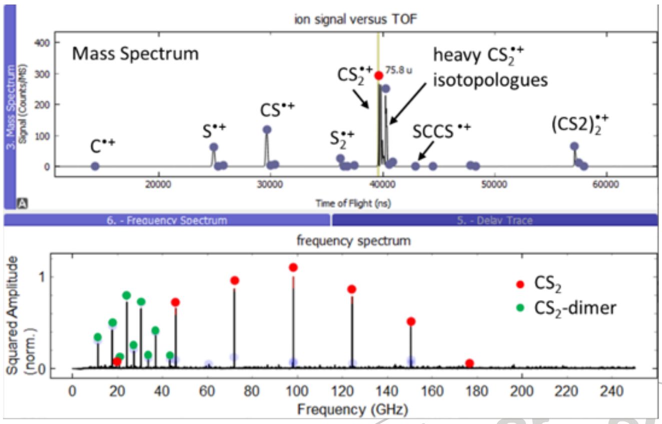


Fig. 1: (Top) Mass spectrum of CS$_2$ clusters and fragments. (Bottom) Rotational Raman spectrum correlated with low-mass shoulder of mass 76 u (CS$_2$ mass channel) shows the rotational fingerprint for CS2 monomer and dimer.

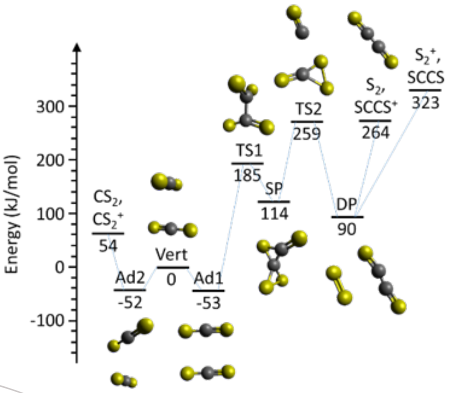


Fig. 2: Calculated minimum-energy path for the formation of cationic CS$_2$-dimer fragments. TS; transition state, SP, DP: spiro and disproportionated intermediates

Symposium : **PHYS1-3**
Recent Trends in Spectroscopy and Microscopy
Room 401+402 THU 16:35
Chair: JunWoo Kim (Chungbuk National University)

Excited-State Reductive Elimination Reactions of Organometallic Complexes

Kiyoung Park

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

Reductive elimination (RE) reactions are often rate-determining steps in catalytic cycles, having transition metal centers serving as active sites that undergo two-electron reduction upon coordinated coupling substrates forming a covalent bond. To define electronic structural factors that determine RE activities, we have characterized high-valent and divalent nickelacycles and binuclear Pd complexes by employing diverse transition-metal-based spectroscopic techniques, such as magnetic circular dichroism, electron paramagnetic resonance, resonance Raman, and X-ray absorption spectroscopies. We have discovered that C□ X bond-forming RE rates are strongly correlated to C/X-to-metal charge-transfer (CT) transition energies, suggesting that the kinetic barrier of the RE reaction is determined by energy cost for internal CT from coupling substrates to the metal center. Using the fact that CT electronic transitions by light mimic the ICT processes of RE reactions, we have examined the RE activities of CT excited states and revealed that compared to the ground state, CT excited states can accelerate RE reactions by up to five orders of magnitude. Furthermore, for divalent organonickel systems, which are majorly utilized as photocatalysts, we have found that unlike what had been proposed in literature, the triplet C-to-Ni CT excited state can be reached via ligand field transitions and induce Ni-C bond homolysis due to its repulsive nature and that the reactivity of the resulting Ni(I) species determines the products of the overall reaction. Our mechanistic studies of ground- and excited-state RE reactions well demonstrate that the electronic-structure level understanding can provide significant insights for developing new chemistry.

Symposium : **PHYS1-4**

Recent Trends in Spectroscopy and Microscopy

Room 401+402 THU 17:10

Chair: JunWoo Kim (Chungbuk National University)

Wide-field nano-spectroscopic imaging microscopy for discovering novel photonic properties of lanthanide nanomaterials

Sang Hwan Nam

Korea Research Institute of Chemical Technology, Korea

Lanthanide nanomaterials with unique photophysical properties are highly regarded as essential new materials for high-tech industries such as photonic devices and intelligent applications. In particular, the novel emission characteristics of lanthanide-doped upconversion nanomaterials (UCNPs) have been revealed by understanding the energy transfer mechanism between the doped ions occurring inside single UCNPs. It is essential to closely analyze and understand the spectroscopic characteristics of the nanomaterials so that they can be manipulated as desired. We built the wide-field nano-spectroscopic imaging microscope and investigated the spectroscopic luminescence properties of Yb^{3+} (sensitizer), Tm^{3+} (emitter)-doped UCNPs over a wide range of irradiance at the single-nanoparticle level. We figured out that the UCNPs have universal emission properties at the same concentration of emitter doping ion, completely excluding the size dependence. Based on these findings, we presented the optimal doping concentration and visualized single UCNPs at an ultra-low irradiance (4.9 W cm^{-2} at 800 nm and 98 W cm^{-2} at 450 nm, respectively), which are five to seven orders of magnitude smaller than those reported in previous studies. And also, we demonstrated omnidirectional CW-upconverting microlaser with ultralow-threshold (0.83 W cm^{-2}) through whole-cavity excitation. Spectroscopic analysis was performed according to the collection position and excitation intensity to understand the emission characteristics exhibited by the whole cavity excitation. Advances in nano-spectroscopic imaging microscopy techniques are expected to accelerate the emergence of lanthanide-based nanophotonics with improved and breakthrough performance.

Symposium : **PHYS1-5**

Recent Trends in Spectroscopy and Microscopy

Room 401+402 THU 17:35

Chair: JunWoo Kim (Chungbuk National University)

Development of Three-Dimensional Super-Resolution Imaging Method for Nano-Patterned Semiconductor Wafers

Doory Kim

Department of Chemistry, Hanyang University, Korea

The recent development of super-resolution fluorescence microscopy (SRM) has dramatically improved the resolution of light microscopy to approximately 10 nm, revolutionizing our understanding of the nanoscale world. However, the application of SRM has been restricted to biological samples, and the application of this technique to inorganic materials, including semiconductors, remains challenging. This is due to the lack of fluorophore labeling methods for inorganic materials with high labeling density for nanoimaging. As recent advancements in nanotechnology enable the fabrication of nanometer-scale features in inorganic materials, the need for SRM imaging of inorganic nanomaterials is increasing. Although electron microscopy or scanning probe techniques have been widely used as metrology tools to determine these nanostructures, the examination of detailed surface chemical composition using these techniques has been limited due to their low molecular specificity. Additionally, high-throughput imaging or 3D imaging for deep layers is often limited with these techniques because of the requirement for an ultrahigh vacuum system and a limited z-scanning range.In this presentation, I will discuss our technology development of a novel approach for highly dense, material-specific fluorophore labeling methods on silicon-based materials for SRM imaging of semiconductor line patterns by utilizing charge-based interactions. Using super-resolution STORM, we have successfully demonstrated that our approach can selectively probe silica or silicon patterns at nanometer resolution, resolving the closely located line nano-patterns in three dimensions. We anticipate that this new method will be a highly valuable super-resolution imaging tool for various inorganic nanomaterials.

Symposium : **PHYS2-1**

Recent Trends in AI and Computational Chemistry

Room 401+402 FRI 09:00

Chair: Hyun Woo Kim (GIST)

Neural machine translation of atomic environments and its application for retrosynthesis prediction

Juyong Lee

College of Pharmacy, Seoul National University, Korea

Designing efficient synthetic routes for a target molecule remains a major challenge in organic synthesis. Atom environments are ideal, stand-alone, chemically meaningful building blocks providing a high-resolution molecular representation. Our approach mimics chemical reasoning, and predicts reactant candidates by learning the changes of atom environments associated with the chemical reaction. Through careful inspection of reactant candidates, we demonstrate atom environments as promising descriptors for studying reaction route pre- diction and discovery. Here, we present a new single-step retrosynthesis prediction method, viz. RetroTRAE, being free from all SMILES-based translation issues, yields a top-1 accuracy of 58.3% on the USPTO test dataset, and top-1 accuracy reaches to 61.6% with the inclusion of highly similar analogs, outperforming other state-of-the-art neural machine translation-based methods. Our methodology introduces a novel scheme for fragmental and topological descriptors to be used as natural inputs for retrosynthetic prediction tasks.Second, in addition to retrosynthesis prediction, we exploited the resolution and robustness of unique molecular representations, i.e., SMILES and SELFIES (SELF-referencIng Embedded strings), reconstructed from a set of structural fingerprints, which are proposed and used herein as vital representational tools for chemical and natural language processing (NLP) applications. This is achieved by restoring the connectivity information lost during fingerprint transformation with high accuracy. Notably, the results reveal that seemingly irreversible molecule-to-fingerprint conversion is feasi- ble. More specifically, four structural fingerprints, extended connectivity, topological torsion, atom pairs, and atomic environments can be used as inputs and outputs of chemical NLP applications. Therefore, this comprehensive study addresses the major limitation of structural fingerprints that precludes their use in NLP models. Our findings will facili- tate the development of text- or fingerprint-based chemoinformatic models for generative and translational tasks.

Symposium : **PHYS2-2**
Recent Trends in AI and Computational Chemistry
Room 401+402 FRI 09:30
Chair: Hyun Woo Kim (GIST)

Enabling complex catalytic system simulation with machine learning

Geun Ho Gu

Department of energy engineering, Korea Institute of Energy Technology, Korea

A critical challenge in understanding catalysis is the complexity of the catalytic system. While the traditional density functional theory calculations focused on the idealized system with simple surfaces and a small reaction network, the realistic system involves complex catalytic sites, evolving catalytic surfaces, and many potentially active reactions and intermediates. In this regard, Machine learning has had a significant impact on catalysis research by enabling efficient predictions of catalytic properties. The flexible machine learning unravels a complex non-linear correlation between atomic structure and catalytic activity and makes predictions on different catalysts without the need for time-consuming and expensive experimental tests and density functional theory. In this presentation, I will discuss how machine learning can be incorporated to research complex systems which includes understanding the mechanism of the hydrogen evolution reaction on the complex jagged Pt nanowire, performing accelerated screening of complex catalytic materials, as well as addressing the exploding reaction network of large molecule catalysis.

Symposium : **PHYS2-3**
Recent Trends in AI and Computational Chemistry
Room 401+402 FRI 10:00
Chair: Hyun Woo Kim (GIST)

Predicting transition state structure and finding reaction paths via machine learning

Sunghwan Choi

Korea Institute of Science and Technology Information, Korea

In the field of chemistry, the machine learning(ML) technique is actively applied to elucidate or predict chemical properties or phenomena which are not resolved by existing experimental and theoretical tools. A transition state (TS) is a central issue in chemical reactions, however, it is difficult for naive ML approaches to be applied in predicting transition states due to the lack of chemical reaction data. In this work, I will present ML study which predicts transition state structures. From reactant and product structures, the proposed ML model accurately predicts interatomic distances of TS structure without loss of physical constraint. Additionally, it is demonstrated that the trained ML model can be applied to figure out the new and chemically meaningful reaction paths with help of configuration sampling of reactant and product.

Symposium : **PHYS2-4**

Recent Trends in AI and Computational Chemistry

Room 401+402 FRI 10:30

Chair: Hyun Woo Kim (GIST)

Data-driven Materials' Discovery from Experimental Research Data

Hyunju Chang

Chemical Data-driven Research Center, Korea Research Institute of Chemical Technology, Korea

Recently, many data-driven studies have been reported in materials science. Many data-driven studies of materials mainly utilize databases based on first-principles calculations. However, machine learning prediction models from computational data tend to be confined to the limitations of computational properties. To develop new materials, it is necessary to build a machine learning prediction model based on data generated from actual experimental research. In this presentation, we would like to introduce recent works that collect experimental data from the entire material development cycle. First, we built a web-based platform to collect the research data easily and build a machine-learning prediction model from the collected data. As an example, I will discuss the following topics. [1] SnSe-based thermoelectric material development, [2] Reaction condition optimization for non-oxidative conversion of methane, [3] Closed-loop optimization of catalyst for oxidative propane dehydrogenation with CO2. Reference[1] Yea-Lee Lee, Hyungseok Lee, et al, J. Am. Chem. Soc, 144, 13748−13763 (2022)[2] Hyun Woo Kim, Sung Woo Lee, Gyoung S. Na, et al., React. Chem. Eng, 6,235. (2021)[3] Jin-Soo Kim, Iljun Chung, et al., in preparation

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

Carbon Neutrality: The Future of the Chemical Industry to Overcome the Climate Crisis

Room 401+402 FRI 14:30

Chair: Hyun Gil Cha (KRICT)

Molecular Simulation Studies on Materials and Biological Systems

Bong June Sung

Department of Chemistry, Sogang University, Korea

Soft matter is a class of materials that has high bulk modulus and low shear modulus. The soft matter includes various types of systems such as biological and materials systems. In this talk, I will discuss the three important characteristics of soft matter: (1) the non-linear response of soft matter, (2) the universality of soft matter, and (3) the non-equilibrium nature of soft matter. Then, I will present a representative molecular simulation on the soft matter, which are the packaging and the ejection processes of a viral DNA. DNA is a biological polymer chain such that its tremendous conformational entropy leads to a small shear modulus and the DNA also belongs to the soft matter. A viral DNA is usually jammed inside the viral capsid and stays in non-equilibrium states. I will report that such a non-equilibrium nature of the jammed conformation of the DNA inside a virus should be a key to understanding the biological processes of the viruses at a molecular level.

Symposium : **PHYS3-2**

Carbon Neutrality: The Future of the Chemical Industry to Overcome the Climate Crisis

Room 401+402 FRI 15:00

Chair: Hyun Gil Cha (KRICT)

From Carbon to Green

Jongho Lim

Institute of Environmental Science and Technology, SK innovation, Korea

SK innovation has various business areas such as energy, chemicals, batteries, and materials. With the company's new identity of 'from carbon to green', we are actively pursuing carbon neutrality. For example, we are striving to reduce Scope 1 and Scope 2 emissions directly from energy and chemical production to 50% by 2030 against the 2019 baseline, and to achieve net zero by 2050. The battery and material businesses also aim to contribute to reducing carbon emissions by using renewable energy at all global business sites by 2030 and achieve net zero by 2035. Additionally, we want to contribute to global carbon reduction through various low-carbon projects such as plastic recycling, battery metal recycling and CCUS (carbon capture, utilization, and storage). Among the several projects, CCUS is quite essential for accomplishing the goal of carbon reduction. Herein, the CCUS technologies being developed by SK innovation are presented.

Symposium : **PHYS3-3**

Carbon Neutrality: The Future of the Chemical Industry to Overcome the Climate Crisis

Room 401+402 FRI 15:30

Chair: Hyun Gil Cha (KRICT)

Hanwha Solutions' R&D Strategy for Carbon Circulation

JAE HYUNG KIM

Hanwha Solutions Chemical Division, R&D Institute, Korea

Hanwha Solutions announced to participate in the NetZero 2050. Since then, it has actively investigated carbon emission reductions on various production plants involved in catalytic processes, polymer syntheses and compounding & formulation processes, etc. In addition, water electrolysis for green hydrogen production using renewable energies such as solar and wind powers has been researched and developed extensively.

Along with the carbon emission reductions, we have investigated to secure sustainable carbon source from carbon (CO2) vented from petrochemical processes and flue stacks as well as from plastic wastes. Two approaches with the plastic wastes are being explored; one is a pyrolysis oil route which can be further upgated to be fed to naphtha cracker, and the other is a direct gasification route which generates syngas to be processed for various chemicals. Dry reforming of CO2 is one of our major focused research areas on CO2 conversion to chemical products.

Hanwha Solutions is actively collaborating with academic institutes and government-funded national laboratories and is constantly dedicated to making contributions to the NetZero 2050 via the carbon recycling technology which is believed to be resolve the global Climate Change issue.

Symposium : **PHYS3-4**
Carbon Neutrality: The Future of the Chemical Industry to Overcome the Climate Crisis
Room 401+402 FRI 16:00
Chair: Hyun Gil Cha (KRICT)

Sustainability R&D of LG Chem

Noma Kim

Vice President, Head of R&D, Platform Technology Research Center, LG Chem, Korea

Since the adoption of the Paris Agreement in 2015, new regulations on carbon emission reductions have been legislated and existing regulations strengthened. Although the adoption of new regulations presents significant challenges for the chemicals industry, the international goal of carbon neutrality also presents new opportunities and enormous market potential, if the technological challenges can be overcome.

LG Chem (LGC) has announced its goal to achieve ‘Carbon Neutral Growth’ by 2030 and ‘Carbon Neutrality’ by 2050. To achieve this 2030 target, LGC needs to achieve greenhouse emission reduction equivalent to 6 million tons of CO2 against its forecasted emissions in a business as usual scenario.

In this presentation, we will introduce various on-going carbon reduction R&D initiatives including green hydrogen production, carbon capture and utilization and plastic recycling by the Platform Technology Research Center of LGC.

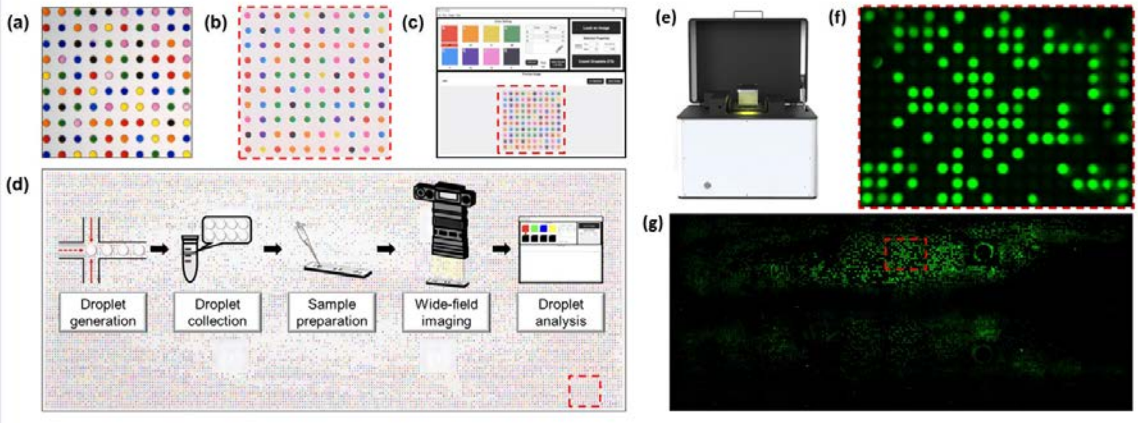
Award Lecture in Division : **ANAL1-5**
Analytical Chemistry for Solving the Social and Industrial Issues
Room 301 THU 17:10
Chair: Sang Yun Han (Gachon University)

Rapid and Accurate Detection of Disease-related Biomarkers at the Single-Molecule Level using Integrated Droplet Microfluidics

Dong-Ku Kang

Department of Chemistry, Incheon National University, Korea

Microcapsule-based microfluidic system (droplet microfluidics, DMF) has been widely utilized for digital analysis to monitor biological molecules at the single-molecule level and Bio-rad digital PCR is the good example of commercially success. DMF-based technologies include various advantages from sample dispersion and compartmentalization that it is due to the dispersion of biomarkers (target) in a single molecule state and the decrease in the concentration of background molecules (noise). In this lecture, we would like to discuss current advances including advantages and challenges in DMF-based technologies and Pro. Kang will also share recent achievements in his laboratory.



Symposium : **ANAL1-1**

Analytical Chemistry for Solving the Social and Industrial Issues

Room 301 THU 15:40

Chair: Seungah Lee (Kyung Hee University)

Next Generation Digital PCR using centrifugal force

Sung Woon Lee

management, RevoSketch Inc., Korea

Currently the most sensitive detection method of gene is digital PCR technology. The digital PCR requires 3 steps to get a result. (1)Partitioning => (2)Amplifying => (3)Read. There are several digital PCR devices in the market and normally using 2~3 devices to perform test and all of them are showing (1)Rain Problem, (2)Liquid Loss, (3)Limited Gene Loading Volume issues. RevoSketch Inc. revealed novel Realtime Digital PCR product digiQuark(TM) to overcome competitor's problem. digiQuark(TM) has advanced features of (1)fully integrated single device, (2)realtime scan operation, (3)scalable structure to adjust total gene loading volume. RevoSketch team developed digiQuark(TM) platform by over 20 years experienced high speed laser fluorescence scanning technology. it is showing best-in-class performance and could be used for early detection of cancer or AD(Alzheimer's Disease).

Symposium : **ANAL1-2**

Analytical Chemistry for Solving the Social and Industrial Issues

Room 301 THU 16:00

Chair: Seungah Lee (Kyung Hee University)

Improvement of skin efficacy by skin lipid enhancer incorporated-lipid nanovesicles

JunBae Lee

Innovation Lab, COSMAX R&I, Korea

In this talk, I introduce skin lipid enhancer incorporated-lipid nanoparticles (SLE-LNPs) in order to improve skin efficacy. As a skin lipid enhancers (SLE), ceramide and fatty acids were used to improve the dermal delivery of cosmetic formulations. The measurements of particle size distribution and zeta potential of lipid nanoparticles (LNPs) with or without SLE have shown the effect of fatty acids to emulsion stability for 4 weeks. The morphology and structure have been investigated using SAXS and TEM. We demonstrate by both in vitro and in vivo skin penetration studies that SLE-LNPs including both ceramide and fatty acids show much improved penetration depth and faster rate compared to ordinary lipid nanoparticles (LNPs) without SLE as well as LNPs with only ceramide. In addition, as a result of in vivo clinical trials, SLE-LNPs has a statistically significant wrinkle decrease rate and melanin index decrease rate compared to the control group, resulting in a better skin efficacy effect. This result might indicate that SLE-LNPs can effectively interact with the SC, resulting in efficient skin delivery of the active agents such as niacinamide and adenosine, resulting improve skin efficacy. This strategy of incorporating both ceramide and fatty acids in LNPs provides a simple and easy route for the rapid and effective delivery of active ingredients across the skin barrier layer.

Symposium : **ANAL1-3**

Analytical Chemistry for Solving the Social and Industrial Issues

Room 301 THU 16:30

Chair: Hee Kyung Na (KRISS)

Development of an animal-alternative model for safety assessment

Sun-Woong Kang

Korea Institute of Toxicology, Korea

We have established laws to register chemical substances and to evaluate the harmfulness and risks of chemical substances and products containing hazardous chemicals for the purpose of protecting the health of the people and the environment. According to the EU and US government statistics (http://www.usda.gov/, http://eur-lex.europa.eu), over 100 million animals are used for toxicity test each year. Recently, various alternative routes have been suggested to minimize or avoid the animal use in researches. This lecture is aimed at anyone interested in the application of 3D cultured model. It offers insights into a wide variety of strategies applying the principles of 3D culture for efficacy evaluation and toxicity test. The 3D cultures for alternative model will be presented in this lecture.

Symposium : **ANAL1-4**
Analytical Chemistry for Solving the Social and Industrial Issues
Room 301 THU 16:50
Chair: Hee Kyung Na (KRISS)

Mass Spectrometry Imaging Analysis for Precision Electronic Devices Using LDI TOF-MS

Jooyeon Oh

Research and Development, ASTA, Korea

MALDI TOF-MS (matrix-assisted laser desorption ionization-time of flight mass spectrometer) has been traditionally used in the analysis of biomolecules. However, the recent adaptation of this technique for the analysis of OLED (organic light-emitting diodes) materials and devices is a promising development. The use of a high-resolution microscope and laser optical system enables the achievement of a spatial resolution of 5μm, which is particularly advantageous for the analysis of small sample areas. The use of LDI TOF-MS (laser desorption ionization-time of flight mass spectrometer) without a matrix is also a significant advantage for the analysis of OLED materials, as the chromophores that absorb photons can be directly ionized. The mass spectra of cations and anions of OLED materials were used to construct a database for OLED analysis using LDI TOF-MS. This database allows for the identification and differentiation of different structural isomer molecules based on their characteristic fragmentation patterns. By comparing the mass spectra of an unknown sample with those in the database, it is possible to identify the specific OLED material and obtain information about its structural properties. This approach enables a high-precision analysis of OLED materials and devices and can be applied to various industrial fields to investigate structural modifications and degradation mechanisms.

Symposium : **ANAL2-1**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 14:30

Chair: Jeong-Wook Oh (Hankuk University of Foreign Studies)

MitoAtlas, a super-resolution proteome map of mitochondria

Hyun-Woo Rhee

Department of Chemistry, Seoul National University, Korea

Mitochondria is the central organelle of cellular metabolism and controls diverse cellular signaling pathways. Since mitochondrial dysfunctions are deeply related to a diverse spectrum of metabolic diseases, there is a great interest for the cataloging sub-mitochondrial proteome with higher resolution. After the establishment of the super-resolution proximity labeling method (SR-PL, Lee SY et al. J. Am. Chem. Soc. 2017, 139, 3651-3662), our lab and Prof. Jong-Seo Kim's laboratory at SNU has co-initiated MitoAtlas project which catalogues a super-resolution proteome map of mitochondria in human cells. For this project, we constructed 38 stable cell lines which stably express sub-mitochondrial targeted proximity labeling enzymes (APEX2 or BioID) per cell line. From the mass analysis of biotinylated proteins generated in each 38 stable cell lines, total ~13,000 biotin-modified peptide information was collected. Using machine learning-based approach, each biotin-labeled site information can be classified to one of sub-mitochondrial spaces (e.g. matrix, IMS, OMM and non-mitochondria). From this workflow, we could construct MitoAtlas, a super-resolution mitochondrial proteome map of 819 mitochondrial proteins. All MitoAtlas proteins have a clearly designated sub-mitochondrial information and the detailed topological information for transmembrane proteins (i.e. IMM-TM, OMM-TM). Among our findings, we also found that ~90 mitochondrial orphan proteins that have not been characterized as mitochondrial protein in previous studies. Overall, Mitoatlas is the first innovative mitochondrial proteome resource constructed by SR-PL method and we expect that our MitoAtlas (www.mitoatlas.org) will lead to a deeper understanding of mitochondrial biology at the molecular level.

Symposium : **ANAL2-2**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 14:50

Chair: Jeong-Wook Oh (Hankuk University of Foreign Studies)

Supramolecular chemistry for biofunctional materials

Yongju Kim

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

Various biological systems rely on the supramolecular assembly of biomolecules through noncovalent bonds for performing sophisticated functions. Using a supramolecular perspective, we can gain a deeper understanding of intermolecular interaction in drug assembly at aqueous media. This provides an insight into the nanostructure-activity relationship for developing new nanoscale pharmaceuticals, which is essential to modern developments in medicines. Among diverse supramolecular building blocks, the aromatic group can serve as remarkable candidates for the creation of well-defined supramolecular structures owing to their rigidity and the π–π stacking of aromatic groups. Based on the aromatic interactions, I present 2D peptide assembly, tamoxifen-selective fluorescent micelles, biocompatible quercetin derivatives, and selective bacterial regulation via a supramolecular approach to medicinal chemistry, enabling the optimization of molecular designs or delivery systems for bioactive molecules.

Symposium : **ANAL2-3**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 15:10

Chair: Jeong-Wook Oh (Hankuk University of Foreign Studies)

Developing an Affordable Nucleic Acid Extraction and RT-PCR Kit for Large-Scale Surveillance of Vector-Borne Viruses: Challenges and Solutions

Kibeom Park

R&D center, Invirustech, Korea

Mosquitoes and ticks are major vectors of viral diseases, and detecting viruses in these arthropod populations is crucial for understanding disease transmission and outbreaks. Despite the emergence of newer methods, RT-PCR remains the gold standard for detecting vector-borne viral RNA due to its sensitivity, specificity, and versatility as a molecular technique. This presentation focuses on the nucleic acid extraction kit and RT-PCR kit that we developed for pan-flavivirus and SFTSV, as well as the challenges of scaling up surveillance efforts. We will discuss the protocol we developed and used, which is also utilized by the Korea Centers for Disease Control and Prevention Agency. We will explore the need for affordable and efficient analysis, and highlight the importance of standardizing protocols to scale up surveillance efforts. In this presentation, we will also discuss a case study of a cost-effective and time-efficient diagnostic solution for a large-scale viral surveillance network. Our approach involves integrating RT-PCR with a sample pooling and nucleic acid extraction strategy to detect multiple or single viral targets. This method is optimized for large-scale surveillance field application and provides an efficient way to monitor emerging viruses and gain a better understanding of domestic vector-borne virus ecology.

Symposium : **ANAL2-4**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 15:30

Chair: Jung-Hoon Lee (Soonchunhyang University)

Development of receptor-based biosensor systems

Seung Hwan Lee

Hanyang University, Korea

Humans can perceive external stimuli through receptors of sensory systems. The binding between a receptor and its target molecule initiates signal transduction and eventually transmits it to the brain. Among these sensory receptors, olfactory receptors have been studied extensively after the pioneering work of R. Axel and L. Buck, who discovered that humans have olfactory receptor genes. The olfactory receptors are members of G-protein-coupled receptors and have seven transmembrane domains. Since receptors can recognize their target molecules with specificity, they can be used as sensing materials for biosensors. In this presentation, olfactory receptor-based biosensors will be introduced. Olfactory receptor-derived peptides, olfactory receptor proteins, and mammalian cells expressing olfactory receptors were obtained and assembled with a nanotube-based sensor system or microfluidic platform. The sensitivity and selectivity of the system will be presented, and various methods to detect gaseous molecules in a manner similar to that of the human nose will be discussed. In addition, potential applications of several receptor-based biosensor systems will be discussed in fields such as food, environment, social security, and medical diagnosis.

Symposium : **ANAL2-5**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 15:50

Chair: Jung-Hoon Lee (Soonchunhyang University)

Fundamental identification of signal generation in bioreceptor-modified CNT-FET

Chang-Seuk Lee

Department of Chemistry, Seoul Women's University, Korea

In this study, we aimed to identify the mechanisms of signal generation in bioreceptor-modified carbon nanotube field-effect transistors (CNT-FETs). Bioreceptors, such as DNA aptamers, peptides, enzymes, and proteins, can be used to modify CNT-FET devices and show significant changes in conductance when specific interactions occur between the receptor and target, modulating localized electric potential within the Debye length (known as the gating effect). There are two major ways to modulate the localized electric potential: first, by the gating effect of charged target molecules, and second, by the gating effect of charged receptor molecules, which can change their conformation after specific binding reactions with target molecules. DNA aptamers, in particular, have unique conformational and orientational characteristics that can be altered by introducing target molecules, which can further modulate the electrical potential of CNT-FET devices.To explore the mechanisms of signal generation in bioreceptor-modified CNT-FETs, we tested two different cases of DNA aptamer-modified CNT-FETs as biosensors with (i) a functionalization method and (ii) different lengths of DNA aptamers with different conformations. The results of these cases showed potential in explaining the fundamental idea of signal generation in bioreceptor-modified CNT-FETs.

Symposium : **ANAL2-6**

Current trends in Biosensors for Disease Diagnosis

Room 301 FRI 16:10

Chair: Jung-Hoon Lee (Soonchunhyang University)

Plasmonic Effects of Gold Nanocubes

Jeong-Eun Park

Division of Chemistry, GIST, Korea

Plasmonics utilize light-matter interaction at a dimension smaller than the wavelength of light. Due to their flexible shapes and geometries, metal-based plasmonic materials can be a reliable tool for obtaining desired plasmonic near- and far-field properties. We first developed a controlled synthesis of gold nanocubes in a highly uniform manner. From their uniform structures and strong plasmonic effect, we achieved reproducible surface-enhanced Raman scattering signals having enhancement factor distribution within 1 order of magnitude. Then by changing the shape of the particles to a core-gap-shell structure, we have induced plasmon hybridization that supports super-radiant plasmon modes. The cube-in-cube nanoparticles have shown the highest metal photoluminescence quantum yield without photobleaching or photoblinking.

Symposium : **LIFE1-1**
Recent Advances in Aging and Reverse Aging
Room 207 THU 15:40
Chair: Young-Tae Chang (POSTECH)

Senescent Cells: A source of systemic aging factors

Ok Hee Jeon

Department of Biomedical Sciences, Korea University of College of Medicine, Korea

Aging is the largest risk factor for many chronic diseases. Studies of heterochronic parabiosis (the surgical joining of young and old mice, in which blood, organs, and environments are shared) rejuvenate old tissues while aging young tissues. Interestingly, using heterochronic blood exchange without organ sharing, the negative influence of the aged circulation was as great as, or more, than the benefits of young circulation, particularly for the liver and brain. While several tissues were studied in blood heterochronicity experiments, the underlying mechanisms of how bloodborne factors promote aging remain largely unknown. Cellular senescence is a response to stress and damage that increases with aging. Senescent cells (SnCs) cease proliferation and secrete multi-faceted senescence-associated secretory phenotype (SASP) proteins. This talk will cover the effects of SnCs that are induced by normal aging and circulating SASP factors in old mice on the systemic induction of senescence and aging in young animals. Specifically, using heterochronic blood exchange in mice, aged mouse blood induced senescence in cells and tissue of young skeletal muscles. We showed that senescence is not a cell-autonomous process and is induced by old blood in young animals with their long telomeres, undamaged DNA, etc. youthful cells and bodies, which is a novel paradigm of relative aging that is uncoupled from the progression of chronological time. In addition, clearing SnCs that accumulate with age accumulated rejuvenates old circulating blood and improves the health of skeletal muscle tissues. Overall, mammalian aging appears to be driven by the excess of systemic factors that include SASP, and the attenuation or removal of these factors is expected to yield new therapeutic strategies for tissue rejuvenation and health span extension.

Symposium : **LIFE1-2**
Recent Advances in Aging and Reverse Aging
Room 207 THU 16:10
Chair: Young-Tae Chang (POSTECH)

Controlling cellular senescence for healthy aging

Young-Sam Lee

Department of New Biology, Daegu Gyeongbuk Institute of Science & Technology, Korea

Aging is a progressive physiological change over time and is mainly associated with the decline of biological functions and senescence in an organism. The loss of biological function in cells, the basic units of tissue and organ, can be caused by cellular stresses, including genomic instability, impaired proteostasis, and dysfunctional subcellular organelles, all of which provoke the cessation of cell division and cellular senescence. Senescent cells have a variety of characteristics such as the irreversible arrest of the cell cycle, resistance to apoptosis, increasing activity of senescence-associated β-galactosidase (SA-β-gal), and secretion of a set of various cytokines involving chronic inflammation and structure remodeling, known as senescence-associated secretory phenotypes (SASPs). Although the transient appearance of cellular senescence plays an essential role in tissue remodeling, efficient immune clearance during embryonic development, and after an injury, a loss of proliferation capacity and SASP secretion in chronic senescent cells per se affects the repair of impaired tissues. Therefore, cellular senescence is suggested to be strongly linked with age-associated tissue damage and diseases. In this talk, I introduce the dysfunctional transmission of signals between the cytoplasm and nucleus as a modality of cellular senescence. To overcome cellular senescence, I show our recent work to determine the molecular pathway of triggering cell cycle progression for reversing cellular senescence. Also, I present an example of approaches for discovering a new class of senolytics.

Symposium : **LIFE1-3**
Recent Advances in Aging and Reverse Aging
Room 207 THU 16:40
Chair: Young-Tae Chang (POSTECH)

Reversion of tumorigenesis and aging by a systems biological approach

Kwang-Hyun Cho

Department of Bio and Brain Engineering, KAIST, Korea

Most biological phenomena such as differentiation, tumorigenesis, and aging have been considered irreversible, but it was shown that differentiation can be reversed by introducing four transcription factors. Tumorigenesis and aging are irreversible in natural environments, but historically there were intriguing experimental observations showing that they might also be reversed under certain conditions which we still do not know exactly at a molecular regulation level. On the other hand, owing to the development of systems biology, we can now investigate complex regulatory mechanism within a cell at a precision of controlling gene regulatory networks for cell fate change as we want. Using such a systems biological approach, we might be able to reprogram a cell to transition to a new stable state of our interest and thereby challenge reversing tumorigenesis and aging from a different perspective.

Symposium : **LIFE1-4**
Recent Advances in Aging and Reverse Aging
Room 207 THU 17:10
Chair: Young-Tae Chang (POSTECH)

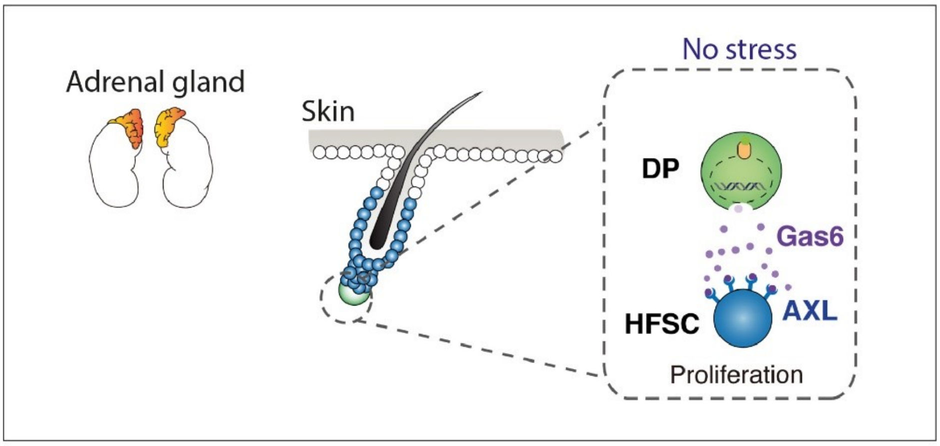
A hair-raising tale: Stress, Aging and Tissue Regeneration

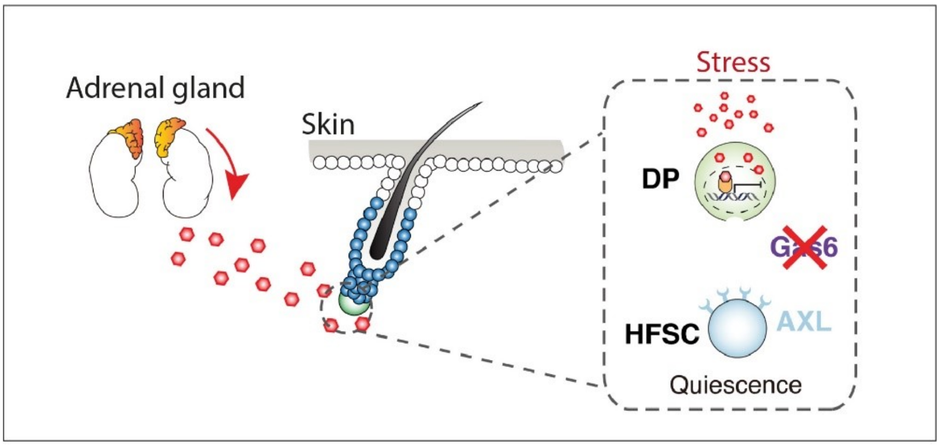
Sekyu Choi

Department of Life Sciences, POSTECH, Korea

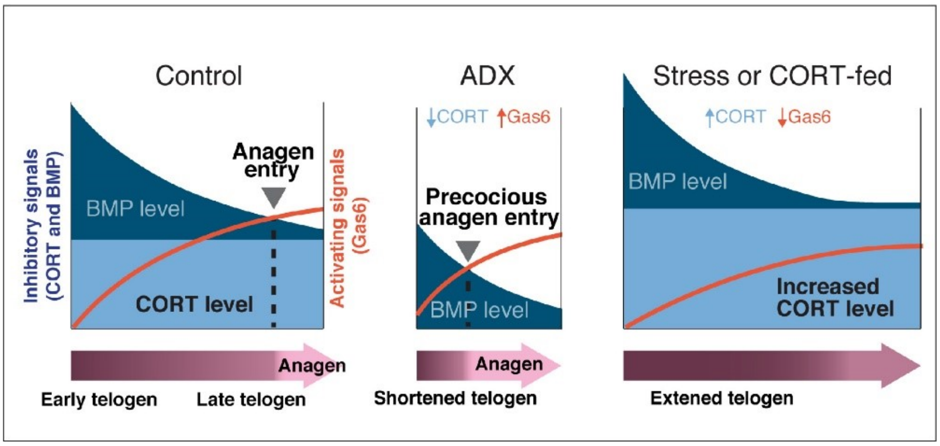
Chronic, sustained exposure to stressors can profoundly impact tissue homeostasis, although the mechanisms by which these changes occur are largely unknown. Here, we report the adrenal gland-derived stress hormone corticosterone (the rodent equivalent of cortisol) regulates hair follicle stem cell (HFSC) quiescence and hair growth in mice. Without corticosterone, HFSCs enter substantially more rounds of the regeneration cycle throughout life. Conversely, under chronic stress, elevated corticosterone levels prolong HFSC quiescence and keep hair follicles in an extended resting phase. Mechanistically, corticosterone acts on dermal papilla (DP) to suppress the expression of a secreted factor, Growth Arrest Specific 6 (Gas6). Restoring Gas6 expression overcomes stress-induced inhibition of HFSC activation and hair growth. Our work identifies corticosterone as a systemic inhibitor of HFSC activity via its impact on the niche, and demonstrates that removal of such inhibition drives HFSCs into frequent regeneration cycles with no observable defects long-term.

Stress hormone maintains hair follicle stem cell quiescence as a systemic factor





Corticosterone and BMPs are two upstream signals to regulate HFSC activity



Symposium : **LIFE2-1**

Sensors and Probes for Bioimaging

Room 207 FRI 09:00

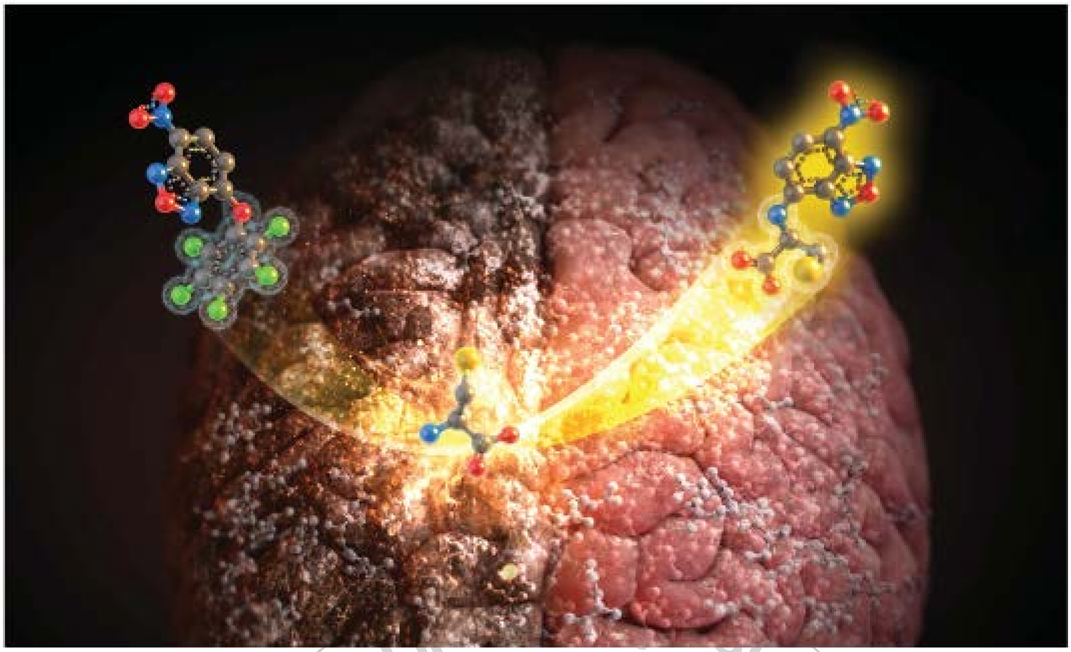
Chair: Jun-Seok Lee (Korea University)

Fluorescent probe for Biothiols and Its Clinical Applications for Real-time Glioblastoma Visualization

Dokyoung Kim

College of Medicine, Kyung Hee University, Korea

Understanding the molecular interactions in biological systems is of fundamental importance. Various types of assay and imaging tools have been developed for studying diverse biological processes. Among these tools, fluorescence-based methods have received significant attention as they enable sensitive detection and imaging by a relatively simple operation. Fluorescent probes with desirable sensing properties (analyte selectivity, sensitivity, bioimaging capability, etc.) are essential for the investigation of molecular interactions and thus have been extensively used in biochemical, clinical, and environmental research areas. In this talk, the speaker will present his multidisciplinary research experiences with key results using fluorescent biothiol probes for clinical applications for real-time glioblastoma visualization. * Topic 1: NBD-pentafluorophenol for cysteine (Cys) sensing (Ref. 1)* Topic 2: NBD-4-hydroxypyridine for homocysteine (Hcy) sensing (Ref. 2)* Topic 3: NBD-2-hydroxypyridine for Cys/Hcy sensing (Ref. 3)References1 An, J. M.; Kim, D. Chem. Sci. 2020, 11, 5658-5668.2 Kim, Y.; Kim, D. Anal. Chim. Acta. 2022, 1202, 339678.3 Kim, D. submitted.



Symposium : **LIFE2-2**
Sensors and Probes for Bioimaging
Room 207 FRI 09:30
Chair: Jun-Seok Lee (Korea University)

Design and synthesis of cancer-related biocomponent-activatable fluorescent probes

Min Hee Lee

Department of Chemistry, Sookmyung Women's University, Korea

Imaging and quantification of specific analytes is essential for a variety of applications ranging from life sciences to the environment. Optical sensing enables non-invasive measurements within biological milieus, parallel monitoring of multiple samples, and less invasive imaging. Among the optical sensing methods currently being explored, small molecule-based fluorescence sensing has received particular attention as a technique with the potential to provide precise, quantitative analysis and real-time fluorescence monitoring. So far, our laboratory has developed a variety of sensing probes using rationally designed activatable fluorophores for sensing, imaging, and biomedical applications. Today, I will talk about development of activatable fluorescent molecules capable of sensing cancer-related enzymes such as nitroreductases, reduced nicotinamide adenine dinucleotide, and reactive oxygen species recently reported in our laboratory. The basic design concepts involving small fluorescent molecules composed of a fluorescent reporter and reactive portion that undergo a selective fluorogenic reaction in response to particular biocomponents will be introduced. In addition, some biological results demonstrating the validation of fluorescent molecules’ operation will be presented in a variety of biological models such as live cancer cells, cancer cell spheroids and tissues.

Symposium : **LIFE2-3**
Sensors and Probes for Bioimaging
Room 207 FRI 10:00
Chair: Jun-Seok Lee (Korea University)

Biomolecular design for control of molecular and cellular communication

Sangkyu Lee

Center for Cognition and Sociality, Institute for Basic Science, Korea

Communication across multiple scales of the biological system, from molecules to organisms, is essential for sharing information among members of a society. At the molecular level, communication among a particular set of molecules is important not only for determining the functions of individual cells but also for creating harmonious and complex multicellular actions, such as brain circuit activity, which ultimately changes organisms' behaviors. Therefore, understanding the impact of molecular communication on higher-level communication is a fundamental step toward explaining how the biological system works as a whole. In the first part of my talk, I will introduce a series of molecular optogenetic tools to control molecular communication in living systems. These optogenetic tools, which use plant photoreceptors, can be applied to a variety of cell types and organisms to control specific molecular functions and corresponding biological processes in a highly spatiotemporal manner. In the second part, I will introduce synthetic approaches for the control of direct cell-cell interactions in the brain. We designed a set of synthetic ligand and receptor proteins to induce direct interaction between neurons and astrocytes, giving astrocytes the capability to prune the target neural circuit. We anticipate that these synthetic approaches will provide unprecedented opportunities to deeply understand the dynamic nature of molecular and cellular communication in a complex biological milieu and their contributions to higher-order biological functions and diseases.

Symposium : **LIFE2-4**

Sensors and Probes for Bioimaging

Room 207 FRI 10:30

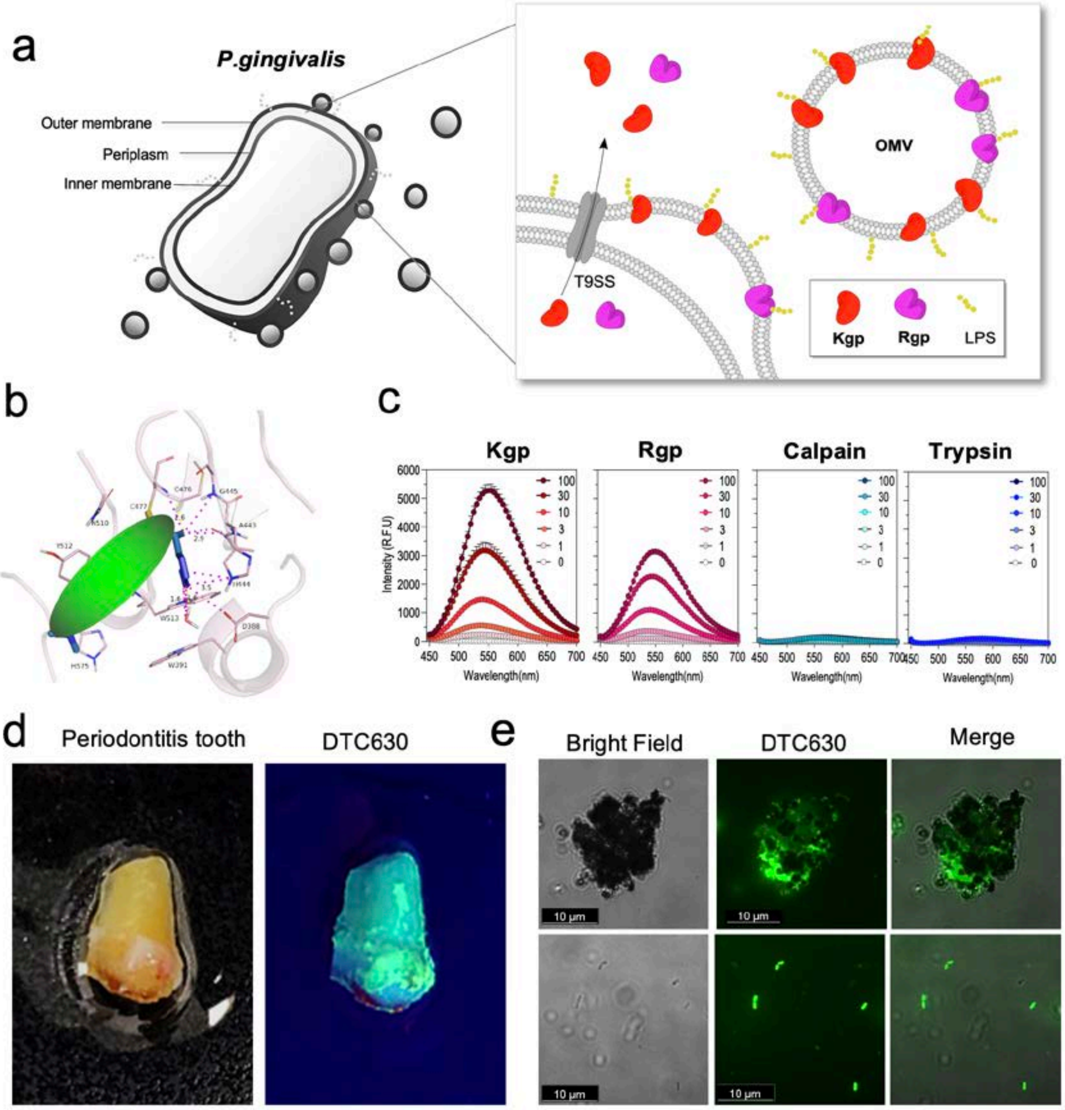
Chair: Jun-Seok Lee (Korea University)

Development of a theragnosis probe for gingipains, cysteine proteases secreted from p. gingivalis

Yun Kyung Kim

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

P. gingivalis is recognized as the major cause of severe and progressive forms of periodontitis in adults. In the gingival tissues, P. gingivalis secretes cysteine proteases, named gingipains. Aided by the proteolytic activities of gingipains, P. gingivalis can invade periodontal tissues through the epithelial barrier and enter periodontal microcirculation where it can then spread through the bloodstream and colonize extra-oral tissues. There is growing evidence of the correlation between P. gingivalis/gingipains and systemic diseases such as cardiovascular disease, rheumatoid arthritis, metabolic disorders, and increased risks of preterm labor. Moreover, P. gingivalis can penetrate to the brain leading to brain inflammation causing Alzheimer’s disease (AD) and Parkinson’s disease-like neuropathology. Therefore, the early detection of gingipains is important to prevent gingivalis-related systemic diseases affecting the whole body. Here we present a fluorescence probe, named DTC630, which is selective for gingipains as its secreted forms or membrane-bound forms. As a fluorescence turn-on sensor, DTC630 switched on its fluorescence, upon binding to the cysteines in the active site of gingipains. By modifying the active site covalently, DTC630 inhibited the proteolytic activity of gingipains, suppressing not only gingipain-induced virulence, but also the growth of P. gingivalis. As a theragnosis probe, DTC630 will be a powerful tool for detecting gingipains in the early state of infection and preventing the survival and invasion of P.gingivalis


a
P.gingivalis
Outer membrane
Periplasm
Inner membrane
T9SS
OMV
Kgp
Rgp
LPS
b
C477
C476
G445
A443
H510
Y512
W513
H444
D388
H575
W391
c
Kgp
Rgp
Calpain
Trypsin
Intensity (R.F.U)
6000
5000
4000
3000
2000
1000
0
100
30
10
3
1
0
450
500
550
600
650
700
Wavelength(nm)
d
Periodontitis tooth
DTC630
e
Bright Field
DTC630
Merge
10 μm

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Award Lecture in Division : **ORGN1-1**
Current Trends in Organic Chemistry
Room 304+305+306 THU 15:40
Chair: Sungwoo Hong (KAIST)

Visible-Light-Induced Photocatalysis

Eun Jin Cho

Department of Chemistry, Chung-Ang University, Korea

Recently, visible light photocatalysis has attracted substantial attention due to its environmental compatibility and mechanistic versatility in promoting a large number of synthetically important reactions. We have developed a variety of radical transformations using Ru-, Ir-, Pt-based photocatalysts and organophotocatalysts either through electron transfer or energy transfer pathway under visible light irradiation. Visible light-induced photoredox methods allowed access to fluoroalkyl group-containing molecules, such as –CF3, –CF2R, –CF2SPh, and –CF2OPh groups. In the studies, electron deficient carbon-centered fluoroalkyl radicals were successfully generated by the appropriate choice of fluoroalkyl source, photocatalyst, additives, and solvent. We studied N-O bond activation via selective energy transfer photocatalysis to generate reactive radical intermediates with the coverage on useful mechanistic insights. More specifically, well-designed N-O bond containing substrates such as 1,2,4-oxadiazolines, oxime esters, and N-indolyl carbonates were successfully utilized in versatile transformations. 1,2,4-Oxadiazolines were converted into spiro-azalactams through iminyl intermediates in the presence of 1O2, benzimidazoles or sulfoximines with external sulfoxide reagent through triplet nitrene intermediates under inert conditions. Besides, oxime esters underwent either intramolecular C(sp3)–N radical-radical coupling or intermolecular C(sp3)–N radical-radical coupling by combined energy transfer-hydrogen atom transfer strategy.

Symposium : **ORGN1-2**

Current Trends in Organic Chemistry

Room 304+305+306 THU 16:10

Chair: Sunwoo Lee (Chonnam National University)

Chiral Molecular Architectures from Helical Foldamers

Hee-Seung Lee

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

Foldamers have gained significant attention in synthetic and biological chemistry as molecular scaffolds that mimic the folding and organizing behaviors of biomolecules. By self-assembling foldamers, complex higher-order structures exhibit interesting physical and optical properties not observed in individual foldamers. In the context of metal-peptide networks (MPNs), foldamers offer a solution to the challenge of creating well-defined chiral channels. The flexible nature of conventional peptide ligands often leads to ill-defined directionality in MPNs, but foldamers allow for the design of well-organized chiral MPNs with various topologies. Additionally, the self-assembly of azo-containing foldamers has also been found to result in distinct morphological and optical properties, offering potential solutions to the limitations of using azobenzene as a fluorescent material in biological systems, such as its low quantum yield and short-wavelength emission. This seminar will cover molecular design strategies for constructing chiral high-order molecular architectures from helical foldamers. (Acknowledgement: This work was supported by the National Research Foundation of Korea, NRF-2018R1A5A1025208).

Symposium : **ORGN1-3**
Current Trends in Organic Chemistry
Room 304+305+306 THU 16:35
Chair: Sunwoo Lee (Chonnam National University)

Guanylurea-containing polymers for intracellular protein delivery

Joong Ho Moon

Department of Chemistry and Biochemistry, Florida International University, United States

The delocalized positive charge on a trigonal planar structure of guanidine creates a unique chemical environment for synergistic ionic, hydrophobic, and hydrogen bonding (HB) interactions with biomacromolecules. Numerous guanidine-containing biomaterials have been developed for the delivery of biologically active substances. However, the same positive charge is also responsible for non-specific interactions with serum proteins and altered cellular entry, resulting in reduced cellular delivery efficiency. The HB interaction of guanidine is also weakened in aqueous environments due to water. In this presentation, our efforts of modulating the guanidine group to achieve high intracellular protein delivery will be presented. Using the reactions between guanidine and isocyanate, various polymers containing guanylurea (GU) groups were synthesized and used for intracellular protein delivery. GU is charge neutral in physiological conditions, and a polymer containing phenyl GU exhibits stable complex formation with various proteins. Apoptosis-inducing enzymes and antibodies were successfully delivered to induce dose-dependent cell viability inhibitions, supporting that the newly developed GU provides chemical environments for non-covalent protein complexation, efficient cellular entry, and the release of proteins to the cytosol.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

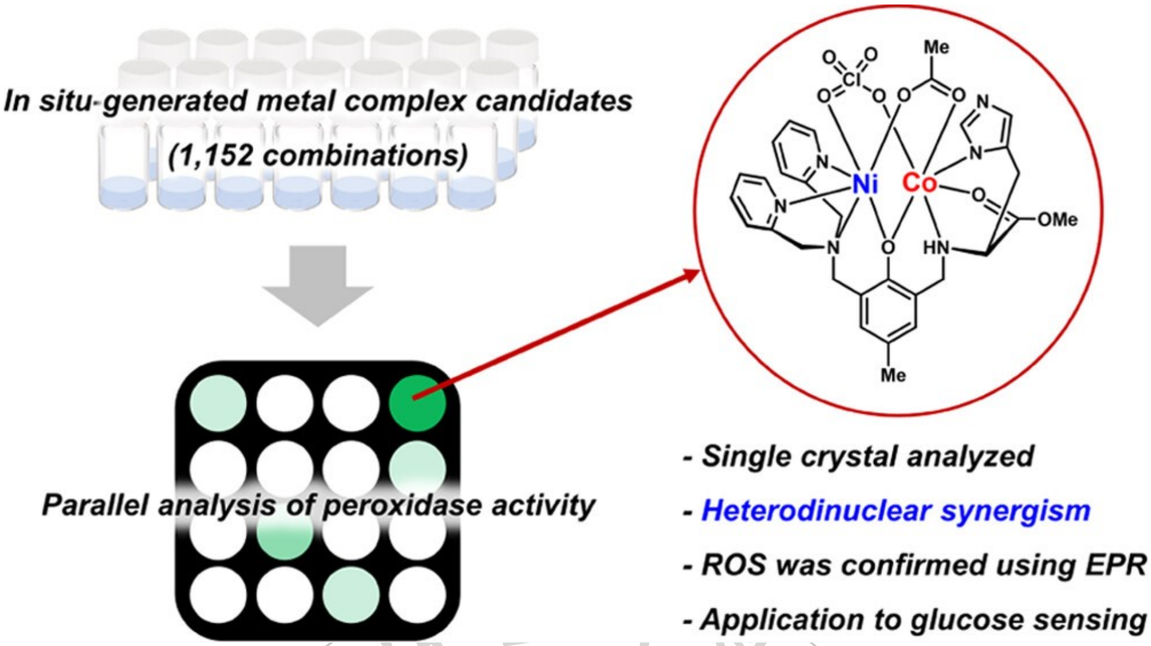
Symposium : **ORGN1-4**
Current Trends in Organic Chemistry
Room 304+305+306 THU 17:00
Chair: Sunwoo Lee (Chonnam National University)

Di-metallic complexes as artificial complex and its application

Min Su Han

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

Horseradish peroxidase (HRP) has been widely used in various fields such as chemical and pharmaceutical industries, the food processing industry, and biosensing systems. Because of its low stability and high preparation cost, the development of artificial peroxidases has attracted great interest. Similar to natural HRP, nanomaterial based-artificial peroxidases catalyze the oxidation of certain substrates in the presence of hydrogen peroxide (H2O2), and have several advantages, including stable storage, inexpensive preparation, and mass production. However, most of these artificial peroxidases work at low pH conditions and relatively high concentration of H2O2, exhibited low reproducibility. Moreover, natural enzymes conjugated with nanoparticles used in fast multi-enzyme cascade reactions show decreased enzymatic activity. To solve these problems, various di-metallic complexes were synthesized as an artificial peroxidase.1 The detailed results and it applications will be presented at this seminar.2.그림 1 삽입 Figure 1. High-Throughput Approach-Based Discovery of a New Hetero-Dinuclear Metal Complex for H2O2 ActivationReferences1. a) S. Kang, B. Y. Park, D. Moon*, M. S. Han*, ACS Applied Materials & Interfaces 2023, 15, 3, 4175-4183. b) Y. Lee, S. Yoo, S. Kang, S. Hong*, M. S. Han*, Analyst, 2018, 143, 1780-1785.2. a) S. Lee, J. Oh, M. S. Han*, ACS Applied Polymer Materials 2023, 5, 1, 67-75. b) S. Lee, M. S. Han*, Chem. Commun., 2021, 57, 9450-9453.


In situ-generated metal complex candidates
(1,152 combinations)
Parallel analysis of peroxidase activity
Ni
Co
OMe
HN
N
O
Me
Cl
- Single crystal analyzed
- Heterodinuclear synergism
- ROS was confirmed using EPR
- Application to glucose sensing

Symposium : **ORGN1-5**
Current Trends in Organic Chemistry
Room 304+305+306 THU 17:25
Chair: Sunwoo Lee (Chonnam National University)

Mild and Efficient Synthesis of Tricyclic Tetrazoles and *N*-Trifluoromethanesulfinyl Ketimines via Cascade Reactions

Chang-Woo Cho

Department of Chemistry, Kyungpook National University, Korea

Methods for synthesizing polyheterocyclic compounds and trifluoromethylthio-containing compounds have been the focus of intensive research efforts due to the structural features and interesting bioactivities of these molecules. Particularly, the development of efficient routes for obtaining these molecules from simple precursors in a single step has become a challenging topic in modern organic chemistry. In this presentation, the cascade diazotization/intramolecular radical C–H heteroarylation of 1-benzyloxy-5-aminotetrazoles and 1-phenethyl-5-aminotetrazoles as substrates using sodium nitrite and acetic acid without heating, catalysis, irradiation, or electrolysis will be discussed. This one-pot reaction afforded the desired tricyclic tetrazole products in good yields without isolation of the diazonium salt intermediate under mild reaction conditions. Furthermore, a new and efficient cascade electrophilic trifluoromethylthiolation/radical rearrangement reaction of ketoximes using *N*-trifluoromethylthio-dibenzenesulfonimide as the SCF_3 source without any additives will also be discussed. This simple one-pot reaction affords the corresponding *N*-trifluoromethanesulfinyl ketimine products in good yields and high *E*-selectivity under mild reaction conditions.

Symposium : **ORGN2-1**
Current Trends in Medicinal Chemistry
Room 304+305+306 FRI 09:00
Chair: In Su Kim (Sungkyunkwan University)

New E3 ligase platforms for PROTAC Technology

Dongyun Shin

College of Pharmacy, Gachon University, Korea

Targeted protein degradation (TPD) is a novel pharmacological modality of drug action which is expected to address the key reason for attrition in clinical trials: lack of efficacy in Phase II. The protein degradation technology can be categorized by what cellular protein degradation processes they use; (1) Proteolysis targeting chimera (PROTAC) degrades the targets by hijacking the cellular ubiquitin-proteasome pathway, and (2) Autophagy-targeting chimera (Autotac) is TPD platform using cellular autophagy-lysosome system. In the context of PROTAC technology, E3 ligases are recruited to the target protein by the ligand component of the PROTAC molecule. The E3 ligase then catalyzes the addition of ubiquitin molecules to the target protein, resulting in its degradation by the proteasome. The specificity of E3 ligase recruitment is a key feature of PROTAC technology, as it enables the selective degradation of disease-causing proteins while sparing healthy proteins. Based on the crystal structure of the CRBN protein, we discovered virtual hits through in silico HTS and determined whether the compounds actually binds to the protein to derive the initial hits by NMR. By analyzing binding mode of proteins and compounds, a new derivative was designed and synthesized to study the structure-activity relationship to derive a novel binder with excellent binding affinity. The derived binders was successfully applied to BRD4 Protac to confirm that the target protein was decomposed. The detailed results will be discussed in this presentation.

Symposium : **ORGN2-2**

Current Trends in Medicinal Chemistry

Room 304+305+306 FRI 09:25

Chair: In Su Kim (Sungkyunkwan University)

Discovery of Novel Protein Kinase Inhibitors as Neurodegenerative Diseases Therapeutics

Jung-mi Hah

Department of Pharmacy, Hanyang University, Korea

Great successes have been achieved in developing small-molecule protein kinase inhibitors as anticancer therapeutic agents. However, kinase deregulation plays essential roles not only in cancer but also in almost all major disease areas, while protein kinase targets in CNS diseases are rarely developed due to the difficulties of common CNS drug discovery. A number of protein kinases are being studied as targets for brain diseases. When developing them, the nature of low-molecular inhibitors-the molecular design that considers cytochrome P450-mediated metabolism, must be accompanied by blood.brain barrier permeability. Degenerative brain diseases and ischemic brain diseases, which are typical CNS diseases, are directly caused by neuronal death, but they are recognized as a result of intracellular signal transduction. Therefore, protein kinase has begun to be studied. The c-Jun N-terminal kinase (JNK) pathway in the MAPK pathway, which is a representative cell signaling system that regulates cell death, has been verified as a target in relation to many diseases. In particular, JNK3 isoform is expressed in brain tissue The distribution is concentrated, and the connection with neuronal death has been studied extensively.Here, we reveal c-Jun N-terminal kinase 3 (JNK3), a protein kinase explicitly expressed in the brain and involved in neuronal apoptosis, with a view toward providing effective treatment for AD. For many years, we have worked on JNK3 inhibitors and have discovered 2-aryl-1-pyrimidinyl-1H-imidazol-5-yl acetonitrile-based JNK3 inhibitors with superb potency ($IC50 < 1.0$ nM) and excellent selectivity over other protein kinases including isoforms JNK1 (>300 fold) and JNK2 (~10 fold). Based on in vitro biological activity and DMPK properties, the lead compounds were selected for further in vivo studies. We confirmed that repeat administration of JNK3 inhibitors improved cognitive memory in APP/PS1 and the 3xTg mouse model.

Symposium : **ORGN2-3**
Current Trends in Medicinal Chemistry
Room 304+305+306 FRI 09:50
Chair: In Su Kim (Sungkyunkwan University)

Prostate-specific membrane antigen (PSMA) and hepsin as biomarkers for metastatic prostate cancer imaging

Youngjoo Byun

Department of Pharmacy, Korea University, Korea

Prostate cancer is the most common type of cancer and the second leading cause of cancer-related death in men. The 5-year overall survival rate for patients with localized prostate cancer in the United States (US) is very high at 97.3%, while it drops significantly to 29% for patients with metastatic prostate cancer.Prostate-specific membrane antigen (PSMA) is a zinc-dependent type II metalloprotease that is highly expressed in most prostate cancers and upregulated in metastatic prostate cacner. PSMA also functions as a receptor and is therefore internalized to the cytosolic region upon binding to a ligand. PSMA-targeted inhibitors were developed by modifying the natural substrates of PSMA, L-aspartyl-L-glutamate and poly-γ-glutamyl folate. The active site of PSMA consists of a pharmacophore S1' pocket, a non-pharmacophore S1 pocket, and two zinc ions in the center. Extensive medicinal chemistry efforts such as bioisosterism and a change in absolute stereochemistry have shown that L-glutamic acid in the S1´ pocket and the urea moiety as a zinc-interacting functional group are best suited to increase PSMA binding affinity. Structural modifications of PSMA-targeted inhibitors have focused on the S1 pocket and the tunnel region. Hepsin is a type II transmembrane protease that is also overexpressed in several cancers, including prostate cancer. Based on the reported hepsin inhibitor Ac-KQLR-ketothiazole, we performed structure-activity relationship studies and identified a Leu-Arg moiety as the minimal scaffold structure for hepsin inhibition. Based on the PSMA-binding ligand and the hepsin-binding ligand, heterobivalent inhibitors targeting PSMA and hepsin have been designed and synthesized.

Symposium : **ORGN2-4**
Current Trends in Medicinal Chemistry
Room 304+305+306 FRI 10:15
Chair: In Su Kim (Sungkyunkwan University)

Decoding mechanism of novel oncogene using small chemical probes

Kyeong Lee

College of Pharmacy, Dongguk University, Korea

The tumorigenic factor AIMP2-DX2, a splicing variant of AIMP2 lacking exon 2 (DX2-here onwards), is often up regulated in many cancers. DX2 plays a critical role in the development of KRAS-driven cancers and acts as a specific regulator of KRAS stability. Heat-shock protein HSP70 was identified as a critical determinant for the cellular levels of DX2. The substrate-binding domain of HSP70 binds to the N-terminal flexible region and GST domain of DX2 stabilizes DX2 and protects it from Siah1 (an E3 ligase specific to DX2)-mediated ubiquitination. Mutational and chemical inhibition of HSP70-DX2 interaction destabilizes DX2, suggesting that HSP70 is functionally significant in maintaining cellular levels of DX2. BC-DXI-495 (IC_{50}= 4.20 μM) and BC-DXI-843 (IC_{50} = 0.92 μM) are small molecules, which binds to DX2 interfering with DX2/HSP70 binding, inducing its degradation via Siah1. SDL01, an allosteric modulator among PPI stabilizers, binds to pocket surrounding the N-terminal flexible region and GST domain of DX2 modulating the structure of DX2 by folding its α-helical loop which stabilizes its interaction with Siah1. BC-DXI-1366 (IC_{50} (1.09 μM) facilitates ubiquitin-dependent degradation of DX2 exhibiting potent inhibitory effects both in vitro and in vivo. Tumor-promoting stabilization mechanism of KRAS via DX2 proposes the interface of the two oncogenic factors as an alternative and effective route to control KRAS-driven cancers. DX2 competitively blocks the access of Smurf2 to KRAS by specifically binds to the hypervariable region and G-domain of KRAS in the cytosol, preventing its ubiquitin-mediated degradation. BC-DXI-32982 (IC_{50} = 0.18 μM) specifically bound to the KRAS binding region of DX2 and inhibits the interaction between these two factors which reduces the cellular levels of KRAS, leading to the suppression of KRAS-dependent cancer cell growth in vitro and in vivo. Collectively, small molecule modulators targeting protein-protein interactions (PPI) of DX2 is considered a promising avenue for cancer therapeutics.

Symposium : **ORGN3-1**
Women Organic Chemists in Korea
Room 304+305+306 FRI 14:30
Chair: Eunsung Lee (POSTECH)

NHC-Catalyzed Regiocontrolled Oxidative Cyclization for the Divergent Synthesis of Aminolactones

So Won Youn

Department of Chemistry, Hanyang University, Korea

Lactones such as phthalides and isocoumarins are one of the significant *O*-heterocycles that exhibit various biological properties and that are utilized as versatile building blocks in organic synthesis. One of the common and straightforward methods for their construction is 5-*exo* or 6-*endo* cyclizations of *o*-alkynylbenzoic acid derivatives through electrophilic activation of the alkyne moiety under transition-metal catalysis or metal-free conditions. Despite the significant advances in this field, achieving high regioselectivity (5-*exo* vs. 6-*endo*) is still a major challenge and the resulting regiochemistry often strongly depends on the nature of the substituents at the alkyne terminus, limiting the diversity of the products. Ynamides are highly useful building blocks for the synthesis of versatile nitrogen-containing molecules. Their intrinsic reactivity results in highly regioselective attack (α-addition) of various nucleophiles to the polarized alkynyl moiety via keteniminium intermediates in the presence of Brønsted/Lewis acid or transition-metal catalyst. In this context, 3-aminoisocoumarins have been synthesized via α-addition of either benzoic acids or benzoates to ynamides. To the best of our knowledge, however, synthesis of phthalide skeletons through β-addition of ynamides has not been developed yet.In this presentation, our recent discovery of NHC-catalyzed regiocontrolled oxidative cyclization reactions of ynamide-tethered benzaldehydes for the divergent synthesis of two different aminolactones from the same substrates will be described. This new method represents a rare example of substrate-independent and regiocontrolled cyclization of alkynes, and furthermore, the first example of NHC organocatalytic cyclization of ynamides bearing a tethered O-Nu instead of metallic and protic acid catalysis.

Symposium : **ORGN3-2**

Women Organic Chemists in Korea

Room 304+305+306 FRI 14:55

Chair: Eunsung Lee (POSTECH)

Ir(NHC)-catalyzed conversion of biomass-derived polyols to fuels and value-added chemicals

Hye-Young Jang

Department of Chemistry, Ajou University, Korea

Transition-metal-catalyzed dehydrogenative reactions using biomass-derived ethylene glycol have received great attention owing to the use of non-fossil fuel resources for the production of useful fuels and chemicals. The catalytic activity of dehydrogenation of ethylene glycol is known to be affected by the ligand structure and metal ions. In particular, iridium complexes coordinated with N-heterocyclic carbene (NHC) ligands are considered efficient catalysts which showed high catalytic activity and stability at even high temperatures. In our research, we synthesized tri-NHC-modified iridium complexes; 1) iridium complexes possessing coordinated two NHC ligands and an uncoordinated imidazolium ion and 2) iridium complexes with tridentate NHC ligands. These iridium complexes exhibited excellent activity in the dehydrogenation of ethylene glycol and subsequent bond formation. Detailed catalytic reaction results and mechanistic studies will be presented.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **ORGN3-3**

Women Organic Chemists in Korea

Room 304+305+306 FRI 15:20

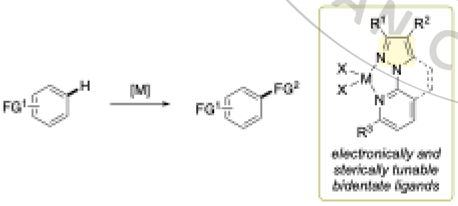
Chair: Eunsung Lee (POSTECH)

Development of New Pyrazole Ligands for Pd-Catalyzed C–H Functionalization

Jung Min Joo

Department of Chemistry, Kyung Hee University, Korea

The development of new ligands and the elucidation of their roles in the catalytic cycle are key to achieving high efficiency and selectivity in transition-metal-catalyzed C–H functionalization. In particular, careful ligand design can enable the functionalization of previously inaccessible substrate positions, which can lead to regiodivergent transformations of common reactants. We have developed a series of pyrazole-containing ligands for nondirected Pd-catalyzed C–H alkenylation, acetoxylation, and deuteration reactions. These studies found crucial factors in the design of ligands for Pd-catalyzed C–H functionalization, which will be useful for further development of new heterocyclic ligands in transition metal catalysis beyond Pd catalysis.



131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

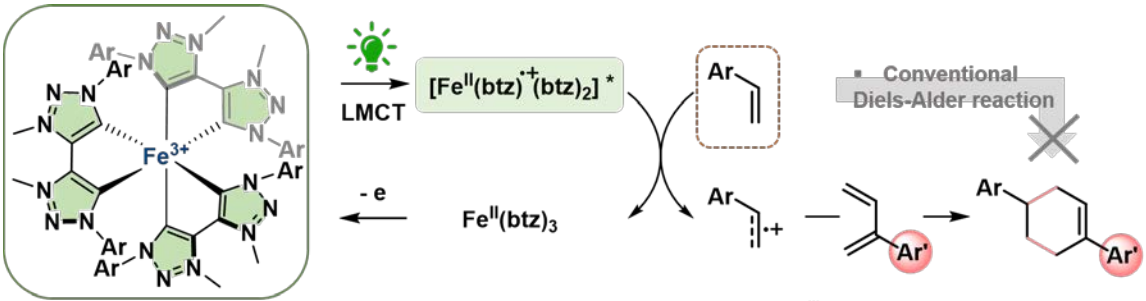
Symposium : **ORGN3-4**
Women Organic Chemists in Korea
Room 304+305+306 FRI 15:45
Chair: Eunsung Lee (POSTECH)

Fe(III)(btz)3 and Fe(III)(phen)3 Catalysis for the Generation of Radical Cation Species of Styrenes and N-Heteroarenes

Eun Joo Kang

Department of Applied Chemistry, Kyung Hee University, Korea

Since the advent of photochemistry, there has been a significant push to replace the photoredox catalysts containing Ru and Ir with those of earth-abundant and sustainable metals; metals such as Cr, Mn, Fe, Co, Ni and Cu are particularly attractive in the first-row transition metals. In classical octahedral polypyridine complexes, RuII and IrIII complexes with the 4d6 and 5d6 valence electron configurations, mainly exhibited the photoactive properties in the metal-to-ligand charge transfer (MLCT) excited states. The analogous MLCT luminescence from 3d6 FeII-polypyridine complexes has been considered attractive, however the more contracted 3d-orbitals of FeII complex effected to result a substantially weaker ligand field than the 4d- or 5d-orbitals. Weaker ligand field on a 3d-metal complexes feature numerous metal-centered (MC) excited states, which allow for a cascade of nonradiative relaxation processes, precluding their use as photocatalysts. In our previous reports on the non-irradiative FeIII(phen)3 catalysis, anethole-type alkenes were singly oxidized to generate radical cations. However, the use of terminal styrenes as alkene substrates presents a unique challenge, due to their relatively high oxidation potentials (Eox = 1.4-1.8 V vs SCE) and propensity for dimerization and polymerization. To date, such challenging terminal styrenes have been oxidized by organo-photocatalysts, p-OMeTPT (Ered = 1.84 V vs SCE) or Mes-Acr+ (Ered = 2.18 V vs SCE) to afford various C-C bond formation reactions, with the requirements of either an electron relay mediator or oxidants. The research presented herein demonstrates the first green-light-driven Fe photoredox system using the Wärnmark FeIII-MIC catalyst with a terminal styrene in radical cationic cycloaddition reactions.



- First C-C bond formation with Wärnmark's $Fe^{III}(btz)_3$ catalyst
- Challenging single-electron oxidation of terminal styrene
- Late-stage cycloaddition of bio-based styrenes

Symposium : **MEDI-1**
The Cutting Edge of Medicinal Chemistry
Room 202+203 THU 15:40
Chair: Hongchan An (KMEDIhub)

Novel drug development and KDDF's supporting strategies

Sun Nam Kim

Korea Drug Development Fund, Korea

Global new drug development trends and future prospects are shared, and points to be focused on in the development of chemical drugs will be explored. In addition, to help universities and the bio industry, the supporting strategy of KDDF (Korea drug development fund), Korea's representative government support program for new drug research and development, will be introduced, .

Symposium : **MEDI-2**

The Cutting Edge of Medicinal Chemistry

Room 202+203 THU 16:10

Chair: Hongchan An (KMEDIhub)

Using radiopharmaceutical imaging drugs for the development of therapeutic drugs: Theranostic lutetium-177-labeled ludotadipep with an albumin binder for prostate cancer

Dae Yoon Chi

FutureChem, Korea

For treatment, radionuclide therapy using α/β-radioisotopes has garnered immense attention in the race to cure prostate cancer since the last decade, especially Ac-225 and At-211 for α -therapy, and Lu-177 for β-therapy. This therapeutic technique is variously called radionuclide therapy (RT), targeted radionuclide therapy (TRT), radioligand therapy (RLT), or protein receptor radionuclide therapy (PRRT). To develop a therapeutic drug for prostate cancer, it is important to develop a molecular imaging agent for determining the therapeutic efficacy of the therapeutic drug. In other words, it is important to develop a molecular imaging agent for PET that can determine the therapeutic efficacy. If the effect of the treatment of cancers can be seen through a molecular imaging agent, the development of therapeutics will be greatly facilitated. We have both radiopharmaceuticals for diagnosis and radiopharmaceuticals for the treatment of prostate cancer. Radiopharmaceuticals prepared in this way are called coupled drugs. The strategy is first to develop radiopharmaceuticals for the diagnosis and then use them to develop a therapeutic drug. We would like to explain and show this strategy in this lecture with a few examples.

Symposium : **MEDI-3**
The Cutting Edge of Medicinal Chemistry
Room 202+203 THU 16:40
Chair: Hongchan An (KMEDIhub)

The immunoproteasome as a novel therapeutic target for Alzheimer’s diseases

Kyung Bo Kim

Department of Cell Biology & Pharmacology, Herbert Wertheim College of Medicine, Florida International University Center for Translational Science (CTS) , United States

With no effective drugs for Alzheimer's disease (AD) in nearly all clinical trials, there is an unmet and urgent need to find a new class of drugs. Unfortunately, a lack of promising new drug targets unrelated to the events leading to the accumulation of the amyloid-beta (Aβ) or tau proteins remains a significant obstacle to developing new drugs. In this talk, we show that the immunoproteasome (iP), an inducible variant of the 20S constitutive proteasome (cP) harboring three immuno-subunits (LMP2, MECL-1, and LMP7), offers a new AD drug target not directly linked to Aβ aggregation and tau polymerization. Specifically, we show that inhibition of iP attenuates cognitive deficits in mouse models of AD in an Aβ independent manner, indicating that the iP-targeting inhibitors hold great promise as a new class of AD drugs that need further investigation in clinical settings. While caution should be used to extrapolate the outcomes in any animal model of AD to patients, we are hopeful that the iP-selective inhibitors warrant further investigations in preclinical and clinical settings and eventually lead to a new, effective therapeutic option for AD patients.

Symposium : **MEDI-4**
The Cutting Edge of Medicinal Chemistry
Room 202+203 THU 17:10
Chair: Hongchan An (KMEDIhub)

A Multiplexed GPCR Screening Platform that Sheds Light on New Biology

Hye Jin Kang

Sungkyunkwan University, Korea

New ligands are discovered through a multiplexed GPCR screening platform, which gives information on novel biology, particularly enlightening of 1) novel itch receptor function and 2) development of new chemogenetic tools. The MRGPRX receptor family (MRGPRX1–4) is a group of mas-related G-protein-coupled receptors that has only recently emerged. MRGPRX2 and MRGPRX4 are two of the most important physiological and pathological mediators of itch and mast cell-mediated hypersensitivity reactions. MRGPRX2 couples to both Gi and Gq in mast cells. We present the creation of effective antagonist probes for MRGPRX2, as well as agonist-stabilized structures of MRGPRX2 bound to Gi1 and Gq in ternary complexes with the natural peptide cortistatin-14 and a synthesized agonist probe, respectively. A particular MRGPRX4 agonist is also described, as well as its structure in a complex with MRGPRX4 and Gq. These discoveries should help speed up the development of structure-guided therapeutics for pain, itch, and mast cell-mediated hypersensitivity.Chemogenetic technologies such as Designer Receptors Exclusively Activated by Designer Drugs (DREADDs) have substantially impacted biological research. Here we will reveal how recent advances in GPCR structural biology and the availability of large libraries of drug-like compounds have allowed us to create new chemogenetic tools and actuators.

Symposium : **MAT1-1**

Recent Trends in Materials Chemistry for Battery Applications

Room 405+406 THU 15:40

Chair: Jongsoon Kim (Sungkyunkwan University)

High-Capacity Ni-rich Cathode Materials for Electric Vehicles

Yang-Kook Sun

Department of Energy Engineering, Hanyang University, Korea

Electric vehicles (EVs) have gained notable market share in recent years largely owing to high energy density and long service life of Lithium-ion batteries (LIBs). However, even EVs that are powered by state-of-the-art LIBs are unable to meet the driving range offered by internal combustion engine vehicles, which is typically 600–800 km. Increasing the driving range of EVs to exceed that of ICEVs requires a substantial improvement in the performance of the cathode, which primarily dictates the energy density and cost of a LIBs. Therefore, recent research on LIBs has focused mainly on development of high-capacity Ni-rich layered LiMO2 (M = Ni, Co, Mn, called NCM or Al called NCA) cathode. To increase the capacity of current NCM and NCA cathodes, the fraction of Ni in the cathodes has been progressively increased. However, such Ni enrichment leads to the rapid deterioration of both the cycle life and the battery safety, which is mainly attributed to microcracking caused by abrupt unit cell contraction during the detrimental H2 - H3 phase transition near charge end. To overcome these limitations, Ni-rich cathode materials must demonstrate mechanical stability and should not exhibit severe microcrack formation even in highly charged states.

In this presentation, to mitigate the tradeoff relationship between reversible capacity and cycling stability, two approaches are introduced. One approach is to develop concentration gradient (CG) cathodes with rod-shaped primary particles that are elongated along the radial direction. High valence Sb doped CG Li[Ni0.9Co0.05Mn0.05]O2 markedly improves the cycling stability of gradient cathodes, retaining ～80% of its initial capacity for 2500 cycles. Another strategy is optimization of both the crystal structure and primary particle morphology by introducing ions with high valence (≥ 5+). The high valence doped Ni-rich cathode demonstrated outstanding capacity retention of 90% after 2000 cycles.

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Symposium : **MAT1-2**
Recent Trends in Materials Chemistry for Battery Applications
Room 405+406 THU 16:10
Chair: Jongsoon Kim (Sungkyunkwan University)

Advanced Design Rules for Polymeric Binders in Next Generation Batteries

Jang Wook Choi

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

Although binder usually accounts for only a small portion of an electrode in rechargeable batteries, its role is becoming more critical as it determines the key performance of the cell. This trend gets obvious in the case of emerging battery systems where the mechanical properties and interfaces are susceptible to damage over cycling. In this presentation, I will introduce my group’s efforts in recent years in developing various binder designs for high-capacity electrodes for Li-ion batteries and emerging post-lithium-ion batteries. For high-capacity Si-based electrodes, binders are based on noncovalent bond-based supramolecular chemistries with the aim of involving self-healing ability. In the second part of my talk, I will also introduce recent efforts along developing advanced binder designs targeting solution-processed sulfide-based all-solid-state batteries. For these series of binders, slurry composition was carefully investigated in conjunction with the polarity of polymeric binder. Various strategies including protection-deprotection chemistry, click chemistry, elastic chain design were applied to address the chemical and physical issues among the electrode components in the sulfide-based all-solid-state batteries.

Symposium : **MAT1-3**

Recent Trends in Materials Chemistry for Battery Applications

Room 405+406 THU 16:40

Chair: Jongsoon Kim (Sungkyunkwan University)

Strategies for Next-generation Rechargeable Batteries with High-Energy-Density

Soojin Park

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

For practical Li-ion battery applications, advanced lithium-ion battery systems are vital to meeting the continuous energy demands and leveling the intermittent and cyclic nature of these energy sources. Here, we present a simple route for synthesizing various dimensional Si materials (such as 2D and 3D). The resulting Si-based anode materials exhibited a long-term cycling stability and excellent rate capability. In addition to Si-based anode materials, using Li metal as an anode in Li-ion batteries is the best way to obtain the high energy density. Many challenges remain such as Li dendritic growth, unstable solid–electrolyte-interphase, and large volume change. We suggest a groundbreaking solution to these challenges consisting in the preparation of a organic and/or organic/inorganic layer. Not only does this protecting layer impede direct contact between electrode and electrolyte, thus avoiding side reactions, but it expedites Li-ion flux in batteries, thus suppressing Li dendrite growth. Notably, protective layer-incorporating Li cells comprising high capacity/voltage cathodes showed highly stable cycling performance in a carbonate-based electrolyte.

Symposium : **MAT1-4**

Recent Trends in Materials Chemistry for Battery Applications

Room 405+406 THU 17:10

Chair: Jongsoon Kim (Sungkyunkwan University)

Porphyrin Catalysis in Reversible Li-Air Breathing Cells

Wonhee Ryu

Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea

Lithium air-breathing batteries (LABs) such as Li–O2 and Li-CO2 batteries, have been recognized as one of the most promising energy storage systems because of (i) application of infinite and easy-accessible air gases as the cathode and (ii) large gravimetric energy densities (> 3500 Wh kg−1) and volumetric energy densities (> 6900 Wh L−1) by the application of lightweight elements such as Li, C, and O. the sluggish reduction and evolution reactions accompanied with solid-to-gas conversion reaction disturb the reversible cell operation during cycling. To address the issues, solid catalyst materials have been introduced to mitigate the low efficiencies of air-breathing batteries. However, they also reportedly promote the decomposition of not only discharge product but also the electrolyte solvent. Furthermore, the limited contact between the solid catalyst and the solid product phase hinders the theoretical catalytic activity for discharge product decomposition. Recently, soluble catalysts or redox mediators (RMs) have attracted considerable attention as promising catalysts for improving LAB performance because of the efficient liquid–solid contact achieved by direct dissolution in the liquid electrolyte and the prevention of passivation by discharge products. Most RMs are mainly based on benzene-ring-containing organic compounds owing to their solubility in organic liquids and extra electrons. However, electron insertion/extraction into/from the benzene ring can affect bonding environments among organic elements, which may destabilize the molecular structure of organic-based RMs during repeated LAB charging–discharging cycles.This study aimed to discover porphyrin-based organometallic compounds that are promising RMs for application to high-performance LABs. Owing to a central metal atom, the proposed RMs exhibited stable electron extraction/insertion, structural stability, high solubility in organic solvents, and auto-oxygenation (or auto-carbon deoxygenation) in ambient air. Our study provides new insights into the introduction of nature-derived porphyrin catalysts and contributes to the development of soluble catalysts for environmental-friendly and cost-effective air-breathing battery technology.

Symposium : **MAT1-5**

Recent Trends in Materials Chemistry for Battery Applications

Room 405+406 THU 17:30

Chair: Jongsoon Kim (Sungkyunkwan University)

Toward the rational design of atomic- and nano-scale defect free Ni-rich layered cathode materials for Li-ion batteries

Hyungsub Kim

Neutron Science Division, Korea Atomic Energy Research Institute, Korea

Ni-rich layered NCM materials have received significant attention as promising cathode materials for Li-ion batteries owing to their high energy density. Although most current research is focused on improving structural stability of Ni-rich layered cathode materials by elemental doping, surface coating, and electrolyte additives, the intrinsic chemical-mechanical instability which is originated from the atomic- and nano-scale defects during the entire synthesis process has not yet been resolved. The simplest way to optimize the electrochemical performance of Ni-rich NCM materials is to tune the crystal structure and redox reaction by controlling the Li content and synthesis temperature. Approximately 1–6 mol% excess Li precursor is commonly used in the synthesis of Ni-rich NCM materials to stabilize the trivalent nickel (Ni^{3+}) in the crystal structure and avoid the formation of the Li-deficient phase $Li_{1-x}Ni_{1+x}O_2$. Also, pre-calcination at 200~500 °C was applied during synthesis to decompose precursor efficiently. However, our understanding of why Li should be overloaded remains incomplete, and there have been no in-depth studies how pre-aging process affects to crystal structure of Ni-rich NCM materials. In this presentation, we investigate atomic- and nano-scale structural evolution of Ni-rich layered cathode using X-ray/neutron scattering and electron/X-ray microscopy. It reveals that excessive Li can be incorporated into TM layer in layered structure by regulating the Li content and synthesis temperature. The pores in primary and secondary particles of Ni-rich cathode were quantified for the first time by using small angle X-ray and neutron scattering analysis, and we propose a simple synthetic route to mitigate the formation of multi-scale defects in Ni-rich NCM cathode with superior electrochemical cycle stability.

Symposium : **MAT2-1**

Current Trends in Materials Chemistry

Room 405+406 FRI 09:00

Chair: Jin Young Kim (KIST)

Semiconductor Nanocrystals: Exploring the chemistry behind different facets

Sohee Jeong

Department of Energy Science, Sungkyunkwan University, Korea

Achieving high-quality and precisely designed semiconductor nanocrystals (NCs) with desirable optoelectronic properties requires a complete mastery over the surface characteristics, which has been a challenging task. In this presentation, I will highlight our contributions to recent progress in this field, which includes the development of a size-dependent shape model and a systematic ligand modification strategy for IV-VI NCs, as well as the achievement of well-defined facets in III-V NCs. First, we discuss the importance of well-defined facets in NCs for enhancing surface control, and how facet-specific surface chemistry has led to comprehensive understanding and control of the IV-VI NC surface. Additionally, we explain the challenges of controlling the III-V NC surface and present a well-defined facets and geometric modulation of III-V NCs. We present a case for using facet-specific chemistry as a platform for mechanistic investigation and materials discovery, which can lead to the development of high-quality and precisely designed NCs for optoelectronic technologies, unlocking new multidisciplinary applications.

Symposium : **MAT2-2**
Current Trends in Materials Chemistry
Room 405+406 FRI 09:30
Chair: Jin Young Kim (KIST)

Growth and Applications of Hexagonal Boron Nitride

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. 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. Finally, the inherent challenges are summarized, and future research directions for the facile CVD-based growth of single-crystal hBN are proposed.

Symposium : **MAT2-3**
Current Trends in Materials Chemistry
Room 405+406 FRI 10:00
Chair: Jin Young Kim (KIST)

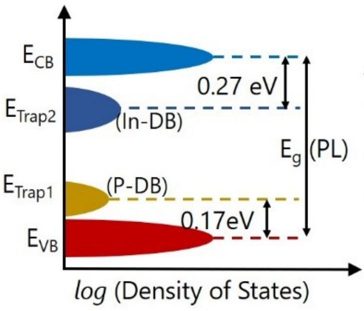
Electronic trap analysis in InP QD optoelectronic devices

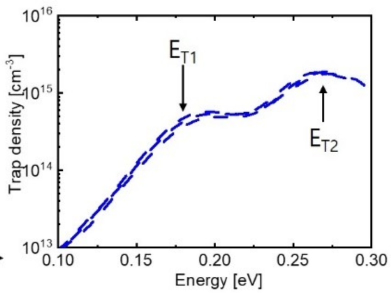
Gyu Weon Hwang

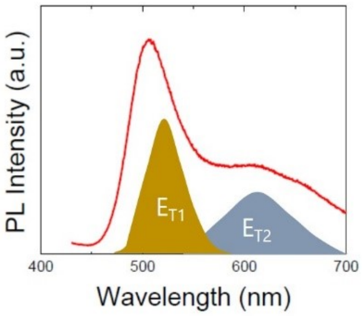
Korea Institute of Science and Technology, Korea

The introduction of QD-LEDs is in line with the current trend in the display industry toward self-emitting displays. Indium phosphide (InP) colloidal quantum dots (QDs) are a popular option for display applications and have optical properties that meet the requirements for a color conversion layer in QD displays. The presence of intermediate gap states or trap states on the QD surfaces negatively impacts the performance and lifetime of QD-LEDs even with various attempts to improve device performance through synthesis methods and surface treatment protocols. The trap state needs to be analyzed in a more thorough way to design a better strategy for the passivation QD surface.

In this study, the InP QD layers were analyzed using an impedance analyzer to investigate the energy level and density of trap states. The study revealed the presence of shallow trap states that were not easily detectable through photoluminescence of InP QD cores. These shallow trap states were found to be related to electronic midgap states originating from P-dangling bonds. Additional impedance analysis results of InP QDs will be presented.







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Symposium : **MAT2-4**

Current Trends in Materials Chemistry

Room 405+406 FRI 10:20

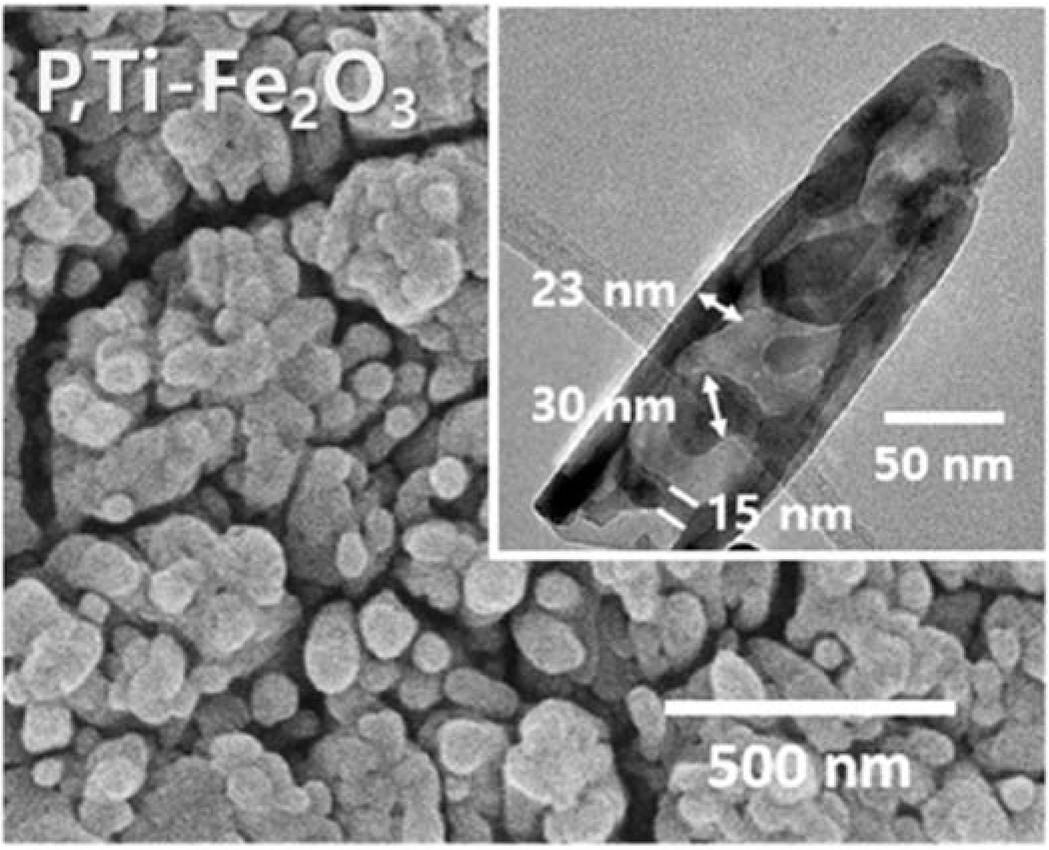
Chair: Jin Young Kim (KIST)

Efficient doping of hematite for water splitting

Ji-Hyun Jang

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

The PEC system utilizes solar energy for electrolysis of water on the surface of a semiconductor photoanode. Hematite (α-Fe_2O_3) proved their potential as a PEC photoanode due to its cost effectiveness and abundance. However, short hole-diffusion length (2-4 nm), poor charge transfer, and sluggish oxygen evolution kinetics have been a chronic bottle neck for the efficient PEC system. In this talk, I will talk about the recent progress on doping of α-Fe_2O_3, which can greatly solve those problems by suppressing the recombination. Especially, I will introduce an in-situ nonmetal phosphorus (P) doping strategy into hematite which not only increases the conductivity by creating oxygen vacancies and internal electric field but also generates a porous structure inside the hematite. Benefiting from the various P doping effects, the resulting P,Ti-Fe2O3 photoanode exhibited 94% improved photocurrent density compared to that of Ti-Fe2O3 (@ 1.23 VRHE) under 1 sun illumination. After applying the co-catalyst, NiFeOx/P,Ti-Fe2O3 showed significantly enhanced photocurrent density with a cathodic shift.


P,Ti-Fe$_2$O$_3$
23 nm
30 nm
15 nm
50 nm
500 nm

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **MAT2-5**

Current Trends in Materials Chemistry

Room 405+406 FRI 10:40

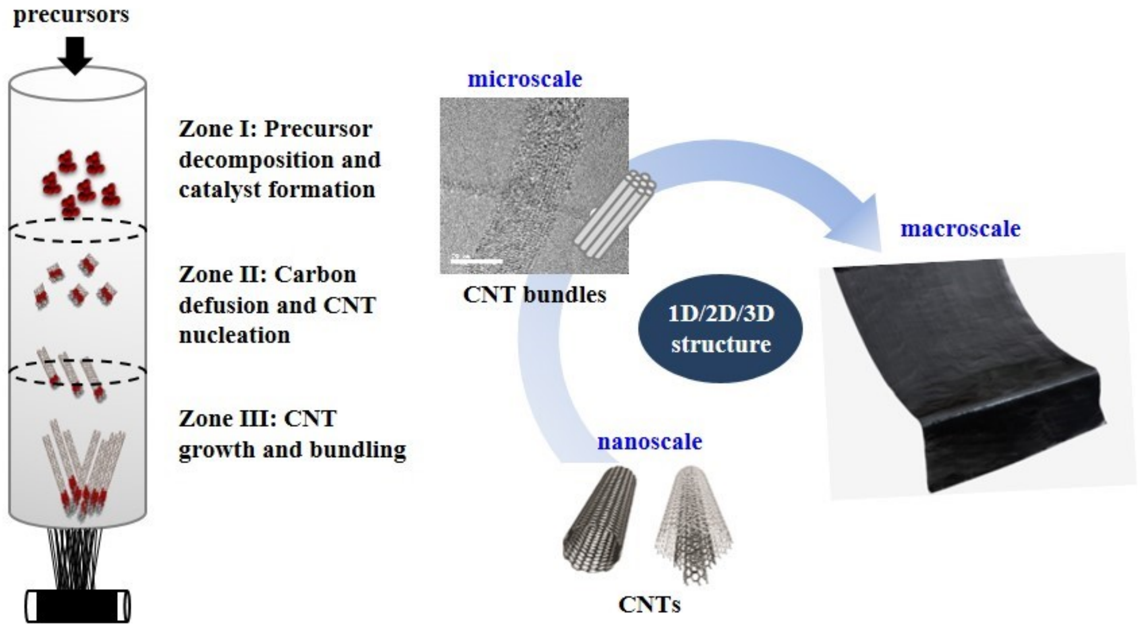
Chair: Jin Young Kim (KIST)

The synthesis of macroscale carbon nanotube structures and their applications

Sook Young Moon

Korea Institute of Science and Technology (KIST), Korea

Carbon nanotubes (CNTs) have been considered for many applications because of their extraordinary physical, chemical, and mechanical properties. Despite their many desirable properties, the short aspect ratio of CNTs hinders their commercial utilization. The synthesis of carbon nanotube's bulk scale structures is major challenges toward future applications. Recent research in the organization of carbon nanotubes into fibers and sheets are mainly reviewed, including methods based on spinning from forests, and direct spinning from the gas phase during synthesis. The floating catalyst chemical vapor deposition (FC-CVD) is an optimum method for bulk production of carbon nanotube. These continuous and scalable one-step production became possible by adding sulfur (S). In this process, the organometallic precursor as a catalyst, and carbon precursor simultaneously pyrolyzed with carrier gases and the residence time in reactor during process is very short which approximately a few seconds. Thus each component, such as catalyst, carbon source, temperature, and carrier gases, strongly affected to final CNT fiber properties. In this study, I will discuss about macro scale organization of carbon nanotubes, including methods based on direct spinning from the gas phase.


precursors
Zone I: Precursor decomposition and catalyst formation
Zone II: Carbon defusion and CNT nucleation
Zone III: CNT growth and bundling
microscale
CNT bundles
macroscale
1D/2D/3D structure
nanoscale
CNTs

Symposium : **MAT3-1**
Display Applications of Inorganic Nanomaterials
Room 405+406 FRI 14:30
Chair: Jiwon Bang (Incheon National University)

High-efficient colloidal InP core-shell quantum dots: synthesis, surface chemistry, and their applications

Jong-Soo Lee

Department of Energy Science and Engineering, DGIST, Korea

Semiconductor colloidal quantum dots (CQDs) have made remarkable progress due to their attractive size-tunable electronic and optical properties, low-cost production, high efficiency, and high stability. In particular, Indium phosphide (InP) quantum dots (QDs) have attracted a great deal of attention in next-generation display technologies, owing to their low intrinsic toxicity and tunable emission from visible to near-infrared region. Despite recent progress in improving the optical properties of InP-based QDs, current synthesis methods have often failed to produce InP QDs with high quantum yield and narrow size distributions, a prerequisite for realizing high color pure emissions. Recently, our group report the importance of precisely controlling the reaction kinetics of InP QDs by a two-step growth process to achieve the narrowest size distribution, engineering the shell coating to reduce interfacial defects for high photoluminescence yield quantum yield (PLQY). In this talk, I will introduce the great synthetic progress of InP core-shell QDs, based on the surface chemistry and the interfacial engineering of InP QDs. By optimizing synthesis conditions, the as-synthesized InP QDs core-multishell exhibited a bright green and red emission with a very high quantum yield and the narrowest emission linewidth of more than 90% and less than 33 nm, respectively.

Finally, I will discuss the challenges related to the recent developments of InP QLED applications and the challenges for achieving high-performance devices.

Symposium : **MAT3-2**

Display Applications of Inorganic Nanomaterials

Room 405+406 FRI 14:55

Chair: Jiwon Bang (Incheon National University)

Colloidal Quantum Dot Heterostructures for Quantum Dot Light Emitting Devices

Byeong Guk Jeong

School of Chemical Engineering, Pusan National University, Korea

Colloidal quantum dots (QDs) have gotten a lot of attention from the display industry due to their exceptional optical properties such as color tunability over the entire visible region, high photoluminescence quantum yield, and pure emission colors with narrow spectral bandwidth. Additionally, the colloidally dispersed QDs enable the solution-based processes to obtain high throughput. Those characteristics lead to QDs into quantum dot light emitting devices (QD-LEDs), which operate under electrical bias, for next-generation display technologies. To enhance the performance of QD-LEDs, developing novel QD heterostructures is required to meet the requirements of the photophysical properties of fluorophores in the devices. Here, I will present the design strategy and synthetic approach of colloidal QD heterostructures for light-emitting devices.

Symposium : **MAT3-3**

Display Applications of Inorganic Nanomaterials

Room 405+406 FRI 15:20

Chair: Jiwon Bang (Incheon National University)

High-Resolution Patterning of Colloidal Quantum Dot Film by Photolithography Process enabled via Atomic Layer Deposited ZnO

Seong-Yong Cho

Department of Photonics and Nanoelectronics, Hanyang University, Korea

Colloidal quantum dot-based light-emitting diodes (QD-LEDs) are one of the potential future self-emissive displays owing to their large-scale solution-processibility and high color purity. For the industrial application of QD-LEDs, high-performance QD-LED and high-resolution patterning of quantum dot (QD) films are required. Photolithography is an ideal tool for patterning QD films. Previously, we have reported the high-resolution patterning of QD films using direct photolithography by ultrathin atomic layer deposition of ZnO on the QD surface. The patterning process is acceptable for Cd-based QD films, but the photoresist severely deteriorates the photoluminescence (PL) intensity of InP-based QD films owing to the presence of sulfonic groups in the photoactive compound. Herein, we report a nondestructive direct photolithography process for QD film patterning using a photoresist that does not affect the PL intensities of Cd- and InP-based QD films. The effect of the photoresist was also verified by a PL lifetime study. Extremely bright Cd- and InP-based QD films were successfully patterned using a softer photoresist, and micropatterning of InP-based QD films is reported for the first time in this work using photolithography. A QD electroluminescence (EL) device was also successfully fabricated using our patterning method and patterned QD EL devices show higher performance compared to reference QD EL devices.

Symposium : **MAT3-4**

Display Applications of Inorganic Nanomaterials

Room 405+406 FRI 15:45

Chair: Jiwon Bang (Incheon National University)

Heteroepitaxial chemistry of zinc chalcogenides on InP semiconductor nanocrystals

Jaehoon Lim

Department of Energy Science, Sungkyunkwan University, Korea

Heterostructured core/shell semiconductor nanocrystals have been widely adopted in light-generating applications to benefit extended photochemical stability and enhanced photoluminescence quantum yield. Here, we analyzed the heteroepitaxial chemistry of zinc chalcogenide on InP semiconductor nanocrystals using zinc carboxylate and trialkylphosphine selenide that are widely used precursors for the synthesis of core/shell heterostructured nanocrystals. The investigation revealed the sterically hindered acyloxytrialkylphosphonium and diacyloxytrialkylphosphorane to be main intermediates in the surface reaction, which retards the metal ion adsorption by a large steric hindrance. The transformation of adsorbates to the crystalline epilayer was disturbed by surface oxides. Raman scattering disclosed the pathway of secondary surface oxidation triggered by carboxylate ligands migrated from zinc carboxylate. A new heteroepitaxy protocol is proposed to fabricate core/shell heterostructured nanocrystals with atomic-scale uniformity of epilayers. Despite the large lattice mismatch of ZnS to InP, we realised the uniform and interface defect-free single ZnS epilayer (~0.3 nm thickness) on the InP nanocrystals, substantiated by the photoluminescence quantum yield of 97.3%. We believe that an understanding of the surface chemistry of heteroepitaxy is crucial for exploring novel synthesis schemes for multifunctional and versatile material libraries made up of heterostructured NCs.

Symposium : **MAT3-5**
Display Applications of Inorganic Nanomaterials
Room 405+406 FRI 16:10
Chair: Jiwon Bang (Incheon National University)

Inkjet printed quantum-dot films formed by controlling surface energy for high-performance color conversion layer

Kwan Hyun Cho

Korea Institute of Industrial Technology, Korea

Self-emissive display such as organic light emitting diodes (OLEDs) and or micro light-emitting diodes (μLEDs) are emerging as promising display technologies due to their high efficiency, higher contrast ratios, and more flexibility. However, there are limitations in fabricating high-resolution pixels and achieving higher color purity in these displays. Quantum dot (QDs) materials are attracting interest in the next generation of displays due to their fascinating properties such as a narrow full width at half maximum (FWHM) and high color purity. In order to achieve high-resolution and high color purity for RGB displays, researchers are exploring the display mode of QD-OLEDs and QD-μLEDs with a quantum dot color conversion layer (CCL) fabricated using inkjet printing (IJP) technology. An inkjet printed quantum dot (QD) color conversion layer needs to be a few micrometers thick to successfully block blue light leaking from the blue OLED or blue μLEDs. Herein, the surface energy of each surface of bank and glass substrate is controlled by using CF4 plasma treatment to control thickness profile and improve color conversion efficiency (CCE) of the inkjet printed quantum dots (QDs) color conversion layer (CCL). The bank surface becomes hydrophobic due to the fluorination, while the glass becomes hydrophilic due to the cleaning effect by the CF4 plasma treatment. Through a systemic investigation of the polar and non-polar components of the surface energy, it is found that the ink behavior of inkjet printed QDs in the pixels is closely related to the non-polar component of the surface energy. In addition, it is found that more rigorous control of the surface is required for array printing and a wide range of thickness profile control is possible by CF4 plasma treatment.

Symposium : **ELEC1-1**
Recent Trends in Electrochemistry-based Energy Storage Researches
Room 205+206 THU 15:40
Chair: Hye Ryung Byon (KAIST)

The effect of cross-talk on the performance of Li-ion batteries and exploiting it for developing high-performance Si-based batteries.

Minkyu Kim

Department of Chemistry, Inha University, Korea

Cross-talk in Li-ion batteries can be defined as the chemical or electrochemical reactions at one electrode affecting the properties of the electrode. Cross-talk in conventional graphite anode-based batteries has been shown to be very detrimental to cell performance such as safety, cycle lifetime, and calendar lifetime. For example, the dissolution of transition metal ions from the cathode and their deposition on the graphite anode is one of the most representative crosstalk behaviors, and it's been widely reported that these deposited transition metal ions lead to impedance rise and electron conduction, resulting in surface parasitic reactions, cracking and pores in the structure of SEI layers of graphite anode. However, graphite anode has been substituted by Si anode as the demand for high-energy-density batteries increases. Therefore, we will face new questions for Si-based batteries: 1) how does crosstalk work in Si-based batteries? 2) what is the effect of crosstalk on cell performance in Si-based batteries?In this talk, I will present an overview of crosstalk in conventional graphite- and Si-based batteries. And I will discuss our recent results showing that crosstalk in Si-based batteries is remarkably different from that in graphite-based batteries and has unexpected beneficial effects to stabilize the SEI of the Si anode. Therefore, crosstalk should be re-addressed in Si-based batteries, and exploiting crosstalk in Si-based batteries can be key for stabilizing the SEI of Si and developing high-performance Si-based batteries.

Symposium : **ELEC1-2**
Recent Trends in Electrochemistry-based Energy Storage Researches
Room 205+206 THU 16:05
Chair: Hye Ryung Byon (KAIST)

Multivalent Non-aqueous Electrolyte and Interface: Understanding and Design

Jaegeon Ryu

Department of Chemical and Biomolecular Engineering, Sogang University, Korea

Multivalent metal (Mg, Ca, Al, etc.) anodes are a game changer to advance the energy density of rechargeable batteries for forthcoming applications with their earth abundance and charge-dense character. However, achieving electrochemical reversibility of multivalent metal plating/stripping is still challenging due to the lack of a 'simple electrolyte' analogous to lithium chemistry and the highly complex nature of electrolyte-electrode interface/interphase. Here, we scrutinize the design of multivalent non-aqueous electrolyte design, interfacial phenomena, and some strategies for the issues.

Symposium : **ELEC1-3**
Recent Trends in Electrochemistry-based Energy Storage Researches
Room 205+206 THU 16:30
Chair: Hye Ryung Byon (KAIST)

Electrochemically driven Thermal Energy Harvesting

Sangtae Kim

Hanyang University, Korea

There has been a few methods to harvest low-grade thermal energy, including thermoelectric devices.Thermal energy harvesting methods via electrochemical means include thermogalvanic cells and thermallyregenerative electrochemical cells, both of which utilize the chemical potential change upon spatial or temporaltemperature gradient. Thermodynamic interpretation of the electrode materials' thermopower reveal thatthermopower is dominated largely by the entropy change associated with temperature gradient, and thus,optimizing the electrode with respect to the entropy change results in improved electrochemically driventhermal energy harvesting. In this talk, I will introduce methods that effectively increase thermopower viaentropy tuning.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **ELEC1-4**
Recent Trends in Electrochemistry-based Energy Storage Researches
Room 205+206 THU 16:55
Chair: Hye Ryung Byon (KAIST)

Impedance imaging: inversion to distribution of diffusion times to diagnose electrode nanostructures

Juhyun Song, Martin Z. Bazant[1,*]

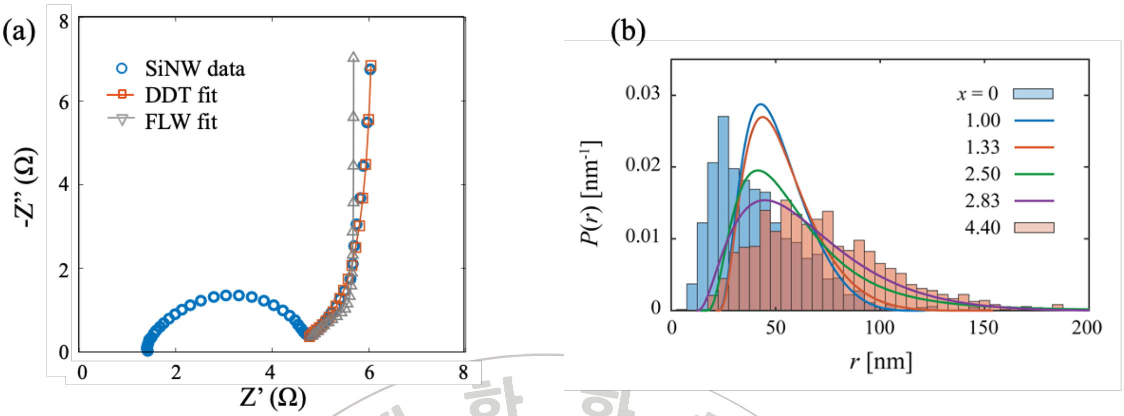
Department of Chemical Engineering and Department of Mathematics, Massachusetts Institute of Technology, Currently at Department of Energy Engineering, Korea Institute of Energy Technology (KENTECH), Korea

[1]*Department of Chemical Engineering and Department of Mathematics, Massachusetts Institute of Technology, United States*

Advanced diagnosis of electrochemical energy systems (e.g., batteries, fuel cells, and capacitors) is becoming increasingly important for their sustainable deployment. In pursuit of higher energy and power density as well as longer lifetime, modern electrochemical energy systems commonly employ nanostructured materials, rendering the transition behavior of finite diffusion impedance now accessible in impedance measurement. The transition spectra are determined by the geometrical randomness of nanostructures, such as particle size distribution in batteries, pore size distribution in capacitors, and distribution of boundary layer thickness in flow batteries. Here we present a diffusion impedance model generalized by a distribution of diffusion times (DDT) to consider the geometrical randomness in common. Not only the model explains a range of deviations from the traditional finite-length Warburg (FLW) with a single diffusion time constant, but it also suggests a nondestructive, global characterization method of the electrode nanostructure by inversely solving the model for the distribution function. Such characterization of nanostructures is particularly essential for diagnosing state-of-health or extent of degradation of electrochemical energy systems. This method is applied to experimental data of a battery, a capacitor, and a flow battery, and their results will be presented.

Figure 1. (a) Impedance spectra of a silicon nanowire (SiNW) electrode at x = 1.33 lithium stoichiometry in silicon. The distribution of diffusion times (DDT) model better fits the low-frequency diffusion impedance compared to the finite length Warburg (FLW) model. (b) Radii distribution of SiNWs at

different lithium stoichiometry (x). Histograms are obtained by analyzing the SEM images at empty and fully-lithiated states, and the curves are obtained by inversely solving the DDT model at the intermediate stoichiometries.



Symposium : **ELEC1-5**

Recent Trends in Electrochemistry-based Energy Storage Researches

Room 205+206 THU 17:20

Chair: Hye Ryung Byon (KAIST)

High Concentration Electrolytes For Lithium And Mulitvalent Batteries

Andrew A. Gewirth

University of Illinois at Urbana-Champaign, United States

In this talk, we discuss results relevant to high concentration (HC) electrolytes and their use in batteries. These electrolytes are evaluated by using vibrational spectroscopy, electrochemical, and force measurements. We show the presence of a surface-confinement effect in the HC electrolytes and the presence of layers, the structure of which changes with applied potential and cation identity. HC electrolytes can be utilized with Li and Na metallic anodes following suitable pretreatment. The presence of divalent or diluent molecules in the electrolyte alters the layering effect. HC electrolytes are utilized in cells with different cathode chemistries. HC electrolyte used with Li2S cathodes is beneficial for achieving high active material utilization, maintaining intimate interfacial contact, and providing buffer space for volume contraction and expansion.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **ELEC2-1**
Recent Trends of Technology & Industry in Major Materials for Secondary Batteries
Room 205+206 FRI 09:00
Chair: Jungdon Suk (KRICT)

Developing High-Energy-Density Solid-State Batteries;From Materials to Cell-level, From Lab to Real Systems

Jihyun Jang

Department of Chemistry, Sogang University, Korea

All-solid-state batteries (ASSBs) are regarded as one of the next-generation technologies that can overcome numerous limitations present in conventional liquid lithium-ion batteries (LIBs) due to their extremely high safety. The comparable performance between the two stems from the development of solid-state electrolytes (SSEs) including sulfide-based SSE such as Li6PS5Cl which possesses an ionic conductivity equivalent to that of liquid electrolytes. However, several challenges must be addressed to achieve the practical application of ASSBs, such as the development of high-performance solid-state electrolytes, stable electrode-electrolyte interfaces, and cost-effective manufacturing processes. This talk will focus on the state of ASSB research, including recent progress in solid-state electrolyte and cathode/anode materials, and cell architecture. In addition, we summarize the recent advancements and highlight the remaining challenges in ASSB research and the advanced cell fabrication processes including the scale-up manufacturing process. We also look into one of the promising alternatives for a highly cost-effective system, Na-ion ASSB, with an outlook on the future of this promising technology.

Symposium : **ELEC2-2**
Recent Trends of Technology & Industry in Major Materials for Secondary Batteries
Room 205+206 FRI 09:25
Chair: Jungdon Suk (KRICT)

Research additives to improve the performance of thick film electrodes

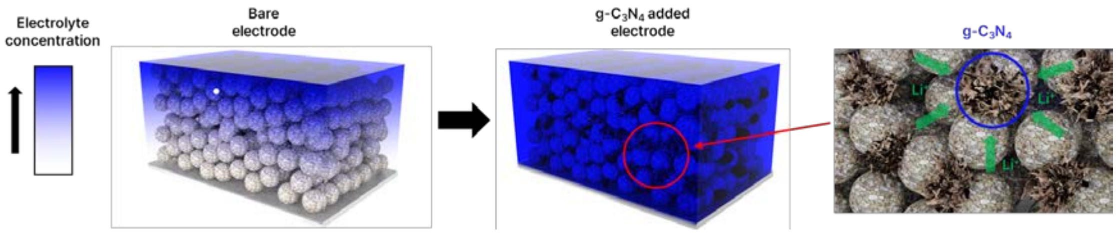
San Moon

Energy Materials Research Center, Korea Research Institute of Chemical Technology, Korea

As the demand for electric vehicles and electronic products continues to rise, there is growing interested in the research and development of lithium-ion batteries (LIBs) that can achieve high capacity and high energy density. To achieve these goals, various methods are used, including improving the characteristics of the active material for the electrode or developing thick electrodes. However, traditionally, thin electrodes have a larger number of sheets in the stack compared to conventional designs, which reduces the loading ratio of active material and makes it difficult to improve energy density compared to thick-film electrodes.

To address this issue, we developed a high-energy-density LIB using thick electrodes, which are capable of storing a large amount of active material. However, as the electrode gets thicker, the concentration gradient of lithium ions at the upper and lower ends of the electrode during charge/discharge testing can lead to the degradation concentration phenomenon and hinder the battery's performance. To solve this problem, we explored using high-content nitrogen-containing N-doping materials as cathode active material additives for thick electrodes. These materials are known for their ability to improve the lithium-ion transfer process and enhance electrochemical performance due to their lithium-ion attraction characteristics and electrolyte wettability improvement, making them an ideal additive for energy storage devices.

Our results show that when the N-doping material additive is applied to the cathode, the capacity of the battery is 74% higher than that of the bare high nickel material, indicating a significant improvement in electrochemical performance. Additionally, we observed a reduction in the lithium-ion concentration gradient problem at the upper and lower ends of the electrode, indicating that the N-doping material effectively addressed the degradation concentration phenomenon.


Electrolyte concentration
Bare electrode
g-C_3N_4 added electrode
g-C_3N_4
Li^+
Li^+
Li^+

Symposium : **ELEC2-3**

Recent Trends of Technology & Industry in Major Materials for Secondary Batteries

Room 205+206 FRI 09:50

Chair: Jungdon Suk (KRICT)

The effect of electrolyte and pressure design for the high performance lithium metal-based batteries

Je-Nam Lee

Korea Electronics Technology Institute, Korea

Lithium metal batteries (LMBs) have been reconsidered to deliver much high energy density beyond current Li-ion batteries. Due to the advantage of Li metal anode, such as high specific capacity (3,860 mAh g^{-1}) and low redox potential (- 3.04 V vs. SHE). However, the most significant barrier is notorious Li dendritic growth, which causes inherent formation of highly porous structures. This porous lithium layer or dead lithium triggers formation of heterogeneous solid electrolyte interfaces (SEI), non-uniform Li+ flux, and uneven volume expansion of the cells. Such problems induces irregular anode swelling, which brings out the degradation of cycle peformance and safety risk. Many different approaches have been proposed so far to control of the Li deposition and suppress the formation and growth of Li dendrites. One of strategies is to build a robust and stable SEI by introducing advanced electrolyte system. Carbonate based electrolyte, which has been used extensively, usually suffer from serious decomposition reactions, which induce Li dendrite growth and short cycle life. Herein, we present ether-based electrolyte system. This newly developed electrolyte system controls interfacial behavior of cathode, which enables high voltage, high capacity of lithium metal batteries. Another strategy is to control of deposition behavior of lithium metal. Lithium-metal batteries in large-scale cells are limited by uneven and excessive anode swelling. To demonstrate the effect of pressure environmetal impact on lithium-metal anode, the distrubition of the actual stack pressure was monitored and the effect of conformal stack pressure system was investigated.

Symposium : **ELEC2-4**

Recent Trends of Technology & Industry in Major Materials for Secondary Batteries

Room 205+206 FRI 10:15

Chair: Jungdon Suk (KRICT)

An industrial researcher’s view about desirable approaches for the development of post lithium ion battery materials

Dongseok Shin

Next Generation Battery Research Center, LG Energy Solution, Korea

During last 30 years, Lithium ion batteries (LIBs) became the dominant solution for the storage of electric energy, owing to their higher energy density and lighter weight comparing with other battery systems, such as lead-acid, Ni-Cd, and Ni-MH batteries. In the meantime, their performances have improved continuously. Nowadays, human beings are enjoying convenient life using diverse portable consumer electronics and electric vehicles adopting advanced LIBs. Although the advancement of technologies for LIBs so far are tremendous, people’s desire to extend interval between charges and immerging technologies such as urban air mobility require batteries with even higher energy density and lighter weight. However, the energy density of current LIBs have been reached close to their theoretical limit. Therefore, many researchers are participating in the research and development of post lithium ion battery technologies and various ideas have been generated and tested. In this talk, desirable approaches for the development of post lithium ion battery materials will be suggested from the view point of an industrial researcher.

Symposium : **ELEC2-5**

Recent Trends of Technology & Industry in Major Materials for Secondary Batteries

Room 205+206 FRI 10:40

Chair: Jungdon Suk (KRICT)

Introduction of Mid/long-term strategies for Future

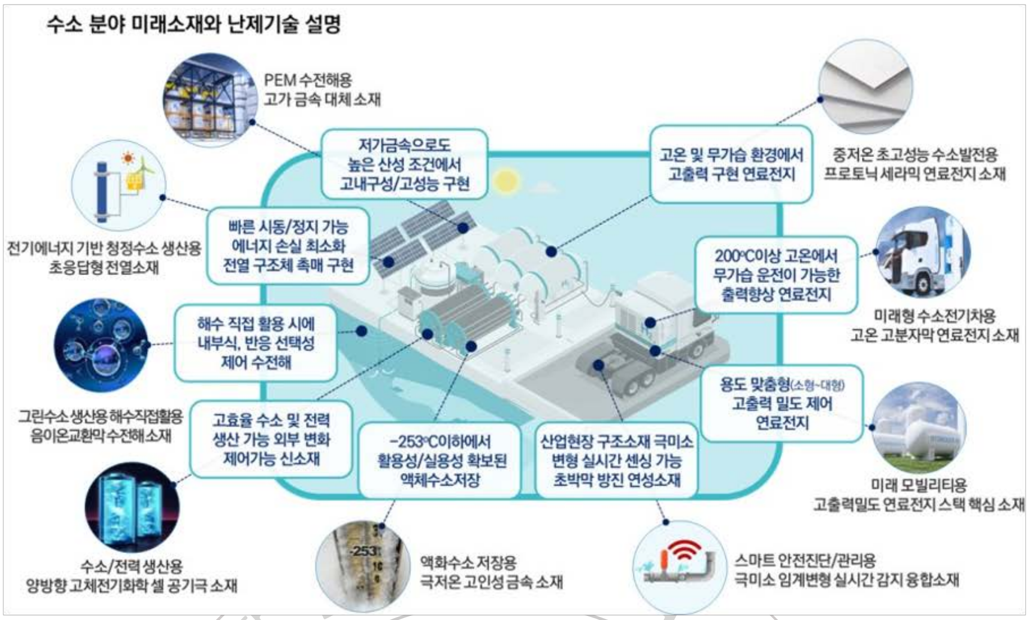
Si-Jin Kim

National Research Foundation of Korea, Korea

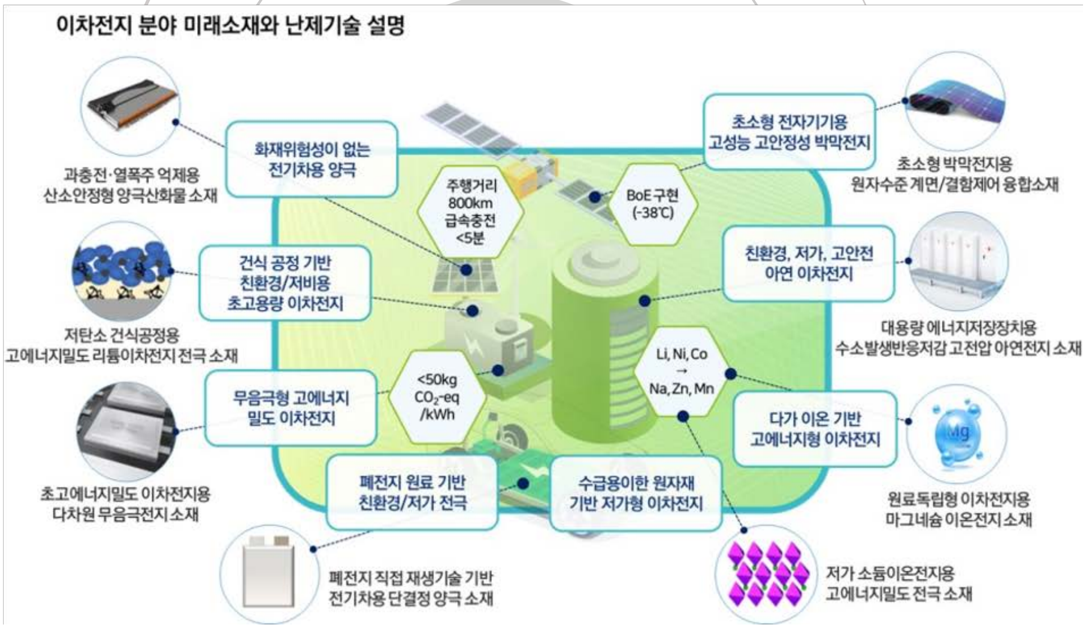
Material R&D('20. Nation 1,724 Billion won /MSIT 32 Billion won) support increased after export regulations. Material R&D has expanded to respond to global supply chain (GVC) reorganization, and related policy development and investment are taking place

By introducing the mid- to long-term strategies and projects of R&D based on the Ministry of Science and ICT, we would like to introduce R&D promotion plans to preoccupy future technologies for next-generation materials

<Future Materials for Hydrogen R&D Category>


수소 분야 미래소재와 난제기술 설명
PEM 수전해용 고가 금속 대체 소재
저가금속으로도 높은 산성 조건에서 고내구성/고성능 구현
고온 및 무가습 환경에서 고출력 구현 연료전지
중저온 초고성능 수소발전용 프로토닉 세라믹 연료전지 소재
전기에너지 기반 청정수소 생산용 초응답형 전열소재
빠른 시동/정지 가능 에너지 손실 최소화 전열 구조체 촉매 구현
200°C이상 고온에서 무가습 운전이 가능한 출력향상 연료전지
미래형 수소전기차용 고온 고분자막 연료전지 소재
해수 직접 활용 시에 내부식, 반응 선택성 제어 수전해
그린수소 생산용 해수직접활용 음이온교환막 수전해 소재
용도 맞춤형(소형~대형) 고출력 밀도 제어 연료전지
고효율 수소 및 전력 생산 가능 외부 변화 제어가능 신소재
-253°C이하에서 활용성/실용성 확보된 액체수소저장
산업현장 구조소재 극미소 변형 실시간 센싱 가능 초박막 방진 연성소재
미래 모빌리티용 고출력밀도 연료전지 스택 핵심 소재
수소/전력 생산용 양방향 고체전기화학 셀 공기극 소재
-253
액화수소 저장용 극저온 고인성 금속 소재
스마트 안전진단/관리용 극미소 임계변형 실시간 감지 융합소재

<Future Materials for LIB R&D Category>


이차전지 분야 미래소재와 난제기술 설명
과충전·열폭주 억제용 산소안정형 양극산화물 소재
화재위험성이 없는 전기차용 양극
주행거리 800km 급속충전 <5분
BoE 구현 (-38℃)
초소형 전자기기용 고성능 고안정성 박막전지
초소형 박막전지용 원자수준 계면/결함제어 융합소재
저탄소 건식공정용 고에너지밀도 리튬이차전지 전극 소재
건식 공정 기반 친환경/저비용 초고용량 이차전지
친환경, 저가, 고안전 아연 이차전지
대용량 에너지저장장치용 수소발생반응저감 고전압 아연전지 소재
Li, Ni, Co → Na, Zn, Mn
<50kg CO₂-eq /kWh
무음극형 고에너지 밀도 이차전지
다가 이온 기반 고에너지형 이차전지
Mg
초고에너지밀도 이차전지용 다차원 무음극전지 소재
원료독립형 이차전지용 마그네슘 이온전지 소재
폐전지 원료 기반 친환경/저가 전극
수급용이한 원자재 기반 저가형 이차전지
폐전지 직접 재생기술 기반 전기차용 단결정 양극 소재
저가 소듐이온전지용 고에너지밀도 전극 소재

Symposium : **ELEC3-1**
Recent Advances in Fundamental Electrochemistry
Room 205+206 FRI 14:30
Chair: Seung-Ryong Kwon (Gyeongsang National University)

Electrochemical study on Contact Electrification

Changsuk Yun

Chemistry, Changwon National University, Korea

Contact electrification is a common physical phenomenon in our daily lives. Recently, many researches have been tried to investigate this charging mechanism at various interfaces. In this talk, I will present the charging mechanism based on electrochemistry and surface analysis at the PDMS/Au interface. The polarity of static charge on a charged Au is inverted to opposite sign after contact with water and the charged Au have reducing power in aqueous phase. I suggest reduction reaction by the charged Au is driven by mechanochemical radicals instead of inverted static charges. Other point in this field is energy conversion based on electrification phenomenon, which is a kind of wasted energy. Thus, I will show that chemical electrification at solid/electrolyte interface can be tuned by energy difference between a self-assembled monolayer/electrode and an electrolyte and demonstrate mechanical-to-electrical energy conversion using a harvester.

Symposium : **ELEC3-2**

Recent Advances in Fundamental Electrochemistry

Room 205+206 FRI 14:55

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Bioelectrocatalytic approaches for bioenergy generation and clean environmental technology

Yoo Seok Lee

Department of Chemical Engineering & Biotechnology, Tech University of Korea, Korea

Bioelectrocatalysis is an emerging and multidisciplinary research topic based on biocatalysis and electrocatalysis. Biocatalysis offers great advantages such as high selectivity, environmental benefits, and broad substrate scope. The advantages of electrocatalysis include the possibility of utilizing renewable electricity as an electron source and high energy conversion efficiency. The synergistic combination of the advantages of biocatalytic and electrocatalytic reactions enables selective biosensing, efficient energy conversion, and synthesis of high value-added chemicals from nitrogen or greenhouse gases. We have focused on studies of enzymatic bioelectrocatalysis, converting nitrogen gas to ammonia, which is the basis for nitrogen fertilizer production and a potential energy carrier in a sustainable future. Although nitrogenase is the only enzyme capable of reducing nitrogen gas to ammonia under mild conditions, it is still energy-intensive, requiring ATP hydrolysis and a reductant. One way to directly reduce the catalytic protein of nitrogenase without ATP hydrolysis is a use of a redox polymer having thermodynamically strong reducing capability. Redox polymer immobilized bioelectrocatalysis facilitates an efficient electron transfer through self-exchange based conduction due to a high effective concentration of catalysts at the electrode surface and more efficient mediation. Recently, we reported MoFe nitrogenase immobilized at an electrode surface with an organic or inorganic redox polymer which is used to reduce the MoFe protein (as a mediator able to transfer the electrons to the MoFe independent of the Fe protein and of ATP hydrolysis) and support the mediated bioelectrocatalysis of N3-, NO2- and N2 to NH3 catalyzed by the MoFe protein. 15N2 labeling experiments and NMR analysis were performed to confirm biosynthetic N2 reduction to NH3.

Symposium : **ELEC3-3**

Recent Advances in Fundamental Electrochemistry

Room 205+206 FRI 15:20

Chair: Seung-Ryong Kwon (Gyeongsang National University)

In-Situ Confocal Fluorescence Lifetime Imaging of Redox-Active Fluorogenic Amplex Red at the Electrochemical Interface

Donghoon Han

Department of Chemistry, The Catholic University of Korea, Korea

Direct imaging of electrochemical processes on electrode surfaces is a central part of understanding spatially heterogeneous electrochemical processes on the surfaces. The redox couple Amplex Red-resorufin exhibits electrofluorogenic properties which are investigated herein by UV-Vis spectroelectrochemistry and electrochemically coupled-fluorescence lifetime imaging (EC-FLIM). The fluorescent resorufin dye is generated at the electrode surface by the irreversible oxidation of the non-fluorescent Amplex Red. Performing EC-FLIM at electrode surfaces allows to monitor spatially resolved electrochemical processes in-situ and in real time. Mapping the fluorescence lifetime of different dimensions by EC-FLIM enables us to reconstruct the relative concentration profile of resorufin on the electrochemical interfaces. In addition, we achieved spatially resolved visualization of the local electrochemical processes occurring on even nanopore electrode arrays as well as conventional microelectrodes, including disk-shaped ultramicroelectrodes and interdigitated array electrodes. This study shows that combining time-resolved fluorescence lifetime imaging with electrochemistry is a powerful tool to study electrochemical reactivity at a spatially resolved level.

Symposium : **ELEC3-4**

Recent Advances in Fundamental Electrochemistry

Room 205+206 FRI 15:45

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Observation and analysis of Pt-Ag alloy nanoparticles using single-entity electrochemistry

Seong Jung Kwon

Department of Chemistry, Konkuk University, Korea

The electrochemical properties of alloy nanoparticles (NPs) consisting of silver (Ag) and platinum (Pt) were analyzed by single-entity electrochemistry (SEE). Each metal component of alloy NP showed different electrocatalytic behaviors towards the hydrazine oxidation reaction compared to the gold (Au). Therefore, when the Pt-Ag alloy NP was investigated using Au ultramicroelectrode by SEE, a different type of current response by each component was observed. A current response consisting of two difference part, called Janus signal, was obtained at appropriated applied potential. The current magnitude ratio of each part in the Janus responses was proportional to the Pt/Ag ratio in the alloy NP. By analyzing the Janus responses from each alloy NP, it was possible to investigate composition ratio as well as the size and concentration of the alloy NP.

Symposium : **EDU-1**

Current Trends in Chemistry Education

Room 204 THU 15:40

Chair: Hyunjung Kim (Kongju National University)

Exploring a new direction for chemistry education in elementary school

Sukjin Kang

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

The Ministry of Education announced the new 2022 Revised Science Curriculum emphasizing to foster students' cross-curricular and general competencies including self management, information processing, creative thinking, aesthetic appreciation, collaborative communication, and community competencies as well as students' domain-specific competencies such as scientific inquiry and problem solving and scientific decision making competencies. In this study, the characteristics of the chemistry-related domain of elementary school science course in the 2022 Revised Science Curriculum are investigated. The 2022 Revised Science Curriculum are characterized by core ideas, three categories of content structure (i.e., knowledge/comprehension, process/skill, value/attitude), achievement standards, and directions for teaching-learning and evaluation, Considerations and suggestions for the future chemistry education in elementary school are discussed.

Symposium : **EDU-2**
Current Trends in Chemistry Education
Room 204 THU 16:05
Chair: Hyunjung Kim (Kongju National University)

Exploring a new direction for chemistry education in secondary school

Jongseok Park

Department of Chemistry Education, Kyungpook National University, Korea

To explore a new direction for chemistry education in secondary school, it's important to consider the current challenges and opportunities in the field. Some possible steps that could be taken include:Incorporating hands-on, inquiry-based learning experiences to engage students in active problem solving and experimentation. Emphasizing the real-world applications of chemistry and its impact on our daily lives. Integrating technology, such as virtual simulations and interactive visualizations, to enhance student understanding and deepen engagement. Providing opportunities for students to collaborate with their peers, build teamwork skills, and develop communication skills. Encouraging students to think critically and independently, and to ask questions and explore their own ideas. Providing ongoing professional development for teachers to keep up-to-date with the latest advancements in chemistry education. Collaborating with industry and academic partners to create opportunities for students to apply their learning in real-world settings. Building a community of learners by promoting student-led research projects, group projects, and science fairs. These steps could help create a dynamic and engaging chemistry education program that prepares students for success in further education and careers in science and technology.

Symposium : **EDU-3**
Current Trends in Chemistry Education
Room 204 THU 16:40
Chair: Hyunjung Kim (Kongju National University)

Leveraging Advanced Technologies for Digital Transformation in Chemistry Education

Byeong-Seon Kim

Department of Chemistry Education, College of Education, Korea

The integration of advanced technologies into education is no longer an option, but a necessity. To shape a desirable future society in the age of artificial intelligence, we need a massive reorganization of systems throughout society. Chemistry education is no exception to this trend, and utilizing the best educational technology is crucial to maximize the potential of every individual through personalized learning. In this context, digital literacy is becoming increasingly important for chemistry education. Advanced technology-based science classes emphasizing digital literacy, including collaboration in classes via cloud, LMX, virtual reality (VR), augmented reality (AR), and virtual experimentation applications, are emerging as powerful tools to enhance digital literacy and provide engaging and interactive learning experiences. By leveraging these tools, chemistry educators can provide students with personalized learning experiences and foster digital literacy, ultimately preparing them for success in a technology-driven society.

Symposium : **EDU-4**
Current Trends in Chemistry Education
Room 204 THU 17:05
Chair: Hyunjung Kim (Kongju National University)

Suggestions for improving chemistry problems in the College Scholastic Ability Test

Jiho Park

Department of Environmental Health, Korea National Open University, Korea

The College Scholastic Ability Test(CSAT) is a tool to measure the scholastic ability required for university education. The basic principle of CSAT is to provide questions that fit the content and level of the high school curriculum and the evaluated students' academic achievement is provided by score.In the CSAT, the science area is divided into four subjects: physics, chemistry, life science, and earth science and the chemistry subject is divided into Chemistry 1 and Chemistry 2, each with 20 questions.The ratio of students took chemistry 1 test among science area 1 in 2023 CSAT is almost half of the ratio in 2013 CSAT. There are the number of opinions brought up for this phenomena, and it is often suggested the the style and contents of the chemistry question needs to be changed to attract the student to choose chemistry subject in CSAT. Some of the recent chemistry questions will be analyzed and the suggested future directions will be discussed.

Symposium : **ENVR-1**
Recent Advances in Recycling Waste Battery
Room 302 THU 15:40
Chair: Hyunwoong Park (Kyungpook National University)

Physicochemical Separation Method for Recovery of Cathode Material and Graphite from Lithium-ion Batteries

Yosep Han

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

Demand for lithium-ion batteries (LIBs) is rapidly increasing due to the increase in electric vehicles and small electronic devices worldwide, and spent LIBs are also rapidly occurring in proportion. Since there is a large amount of valuable materials and spheroidized graphite in LIBs, recycling of LIBs is absolutely necessary in terms of securing raw materials and protecting the environment. A pre-treatment process is required for effective recycling of waste LIBs, and through the pre-treatment process, it is possible to increase the recovery efficiency of valuable materials in LIBs and reduce energy consumption in the subsequent process. In particular, many papers have been published in the past 5 years for effective recovery of cathode material and graphite by physicochemical separation of LIBs prepared by the pretreatment process. Therefore, it would be appropriate to write the review in terms of the latest technologies, mechanisms and prospects for physicochemical separation methods such as classification (i.e., sizing), electrostatic separation, gravity separation and froth flotation. This review, for the first time, provides an in-depth discussion of the physicochemical separation method for the effective recovery of cathode material and graphite in waste LIBs. Acknowledgement: This work was supported by Korea Environment Industry & Technology Institute(KEITI) through R&D Project of recycling development for future waste resources Project, funded by Korea Ministry of Environment(MOE)(2022011144)

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **ENVR-2**
Recent Advances in Recycling Waste Battery
Room 302 THU 16:10
Chair: Hyunwoong Park (Kyungpook National University)

Resource recycling of large capacity lithium ion battery

Hong in Kim

Korea Institute of Geoscience and Mineral Resources, Korea

As the global electric vehicle market soars to 145 million units in 2030, the need for recycling lithium secondary batteries for electric vehicles is increasing. Therefore, studies on the recovery of useful resources from large-capacity waste lithium-ion batteries are being conducted in Europe and China. Large-capacity lithium-ion batteries are becoming an energy source for electric vehicles such as HEV, PHEV, and EV. The weight of lithium-ion battery packs used in electric vehicles ranges from 50 to 400 kg, and the total energy of an electric vehicle is about 4 to 40 Kwh per pack, and about 85 Kwh for Tesla Model S. In general, one pack consists of several modules, and each module consists of several cells, and each cell consists of a negative electrode, a separator, and a negative electrode, and is used as a battery. Lithium secondary batteries for electric vehicles correspond to 4 to 5,000 cell phone batteries, so care must be taken when recycling them, such as fire and explosion, and an efficient pretreatment process must be developed to secure leadership with global lithium secondary battery recycling companies in Europe and China. It will be advantageous to secure. By-products such as aluminum and plastic are difficult to recycle due to their low economic feasibility. The recycling process of lithium ion batteries is largely divided into a dry process and a wet process, which show a big difference in the presence or absence of a pretreatment process, the amount of treatment, process cost, and investment cost, and also show a big difference in the type of recovered metal. This work was supported by the Korea Environmental Industry & Technology Institute (KEITI) grant by the Korea government (Ministry of Environment) (No. 2022003500006, 23-9876).

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Symposium : **ENVR-3**
Recent Advances in Recycling Waste Battery
Room 302 THU 16:40
Chair: Hyunwoong Park (Kyungpook National University)

Current Issues of Recycling Spent Li-ion Batteries and Advanced Recycling Technologies

Jung-Je Woo

Gwangju Clean Energy Research Center, Korea Institute of Energy Research, Korea

The lithium-ion battery (LIB) market is expected to reach 390GWh by 2030, as a result of the expansion of the EV market, which directly causes a significant increase in the amount of spent LIBs [1]. If EVs have a life expectancy of about ten years, the total amount of spent LIBs will amount to 1,000 GWh. The spent LIB poses a risk of releasing dangerous chemical species and posing an explosion risk; some accidents involving significant fires at recycling facilities in the U. S. have been documented [2]. Therefore, the creation of a suitable post-processing method for used LIBs is a critical and urgent issue. The post-processing of used LIBs generally aims to recover valuable metals using pyrometallurgy and hydrometallurgy techniques. The practical recycling processes dealing with several tons of used batteries apply these approaches, which have a high level of maturity. However, harmful pollutants are produced by both hydrometallurgy and pyrometallurgy methods, and they both have low economic viability [3]. Due to this, a lot of researchers are concentrating on how economically viable recycling is becoming. In this presentation, we describe the current state of the battery industry and recycling technologies, a more advanced recycling method (cathode direct recycling), and our research efforts to develope a fundamental technology for inexpensive and environmentally friendly battery recycling. We developed a cutting-edge recycling technology that recovers used Li-ion batteries quickly under mild conditions in order to increase the economic viability of the recycling process. A Li-loss battery's capacity increased from 77.0 to 95.7% after 50 minutes of recovery at room temperature, and it displayed excellent cycling stability over 200 cycles, comparable to a fresh battery.References1. Pillot, C., BATTERIES 2017 (2017)2. Gavin Harper et al., NATURE 575 75-86 (2019)3. Lithium-Ion Battery Recycling: 2 Million Tons by 2030, BloombergNEF (2019)

Symposium : **ENVR-4**

Recent Advances in Recycling Waste Battery

Room 302 THU 17:10

Chair: Hyunwoong Park (Kyungpook National University)

Development of Mass Production Technology for NCM Cathode Precursors Using High-speed Co-precipitation Method and Its Application in Recycled Raw Materials

Jung Hoon Song

LIB Materials Research Group, Research Institute of Industrial Science & Technology, Korea

A precursor manufacturing process widely used in the secondary battery field is CSTR based technology. However, this type of process technology have a disadvantages of long stabilization time as well as low production efficiency for precursor production. In this regard, we will present an efficient synthesis process using a Taylor reactor with a relatively fast mass transfer rate, and introduce a technology as an alternative process . Also, we would like to introduce the development process of scaling up of Taylor reactor from laboratory scale to the mass production scale. In addition, we would like to briefly introduce the results of applying Taylor reactor to the synthesis of secondary battery precursors using recycled metal sulfate raw materials, which have recently become an big issue in Lib research.AcknowledgementThis work was supported by the Project number 20010900 by the Ministry of Trade, Industry and Korea Evaluation Institute of Industrial Technology (KEIT)

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:00

Chair: Jeung Gon Kim (Jeonbuk National University)

Recyclable Poly(*β*-amino ester) Covalent Adaptable Network Composite with High Thermal Conductivity

Dupyo Jeon, Chae Bin Kim*

Department of Polymer Science and Engineering, Pusan National University, Korea

As current electronics get lighter, denser in energy, and being more eco-friendly, relevant industries strive to develop recyclable polymer composite with high thermal conductivity (TC). However, a trade-off between composite weight and TC prohibits constant increase in filler loading. To develop recyclable polymer composite with high TC and lightweight, therefore, a new poly(*β*-amino ester) covalent adaptable network (CAN) was synthesized and composites were prepared by mixing the CAN and *h*BN in powder forms. Ascribing to a unique characteristic of CAN, continuous heat conduction pathways could be well-constructed as the *h*BN was confined between malleable CAN domains. As a result, a TC of 7 W/mK was achieved at only 30 vol% *h*BN, which is 30 vol% less than the loading for composites prepared by mixing liquid monomer and filler. To emphasize efficient recyclability of the composites, composite reprocessing and filler recovery by depolymerizing the matrix in heated water were also demonstrated.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:12

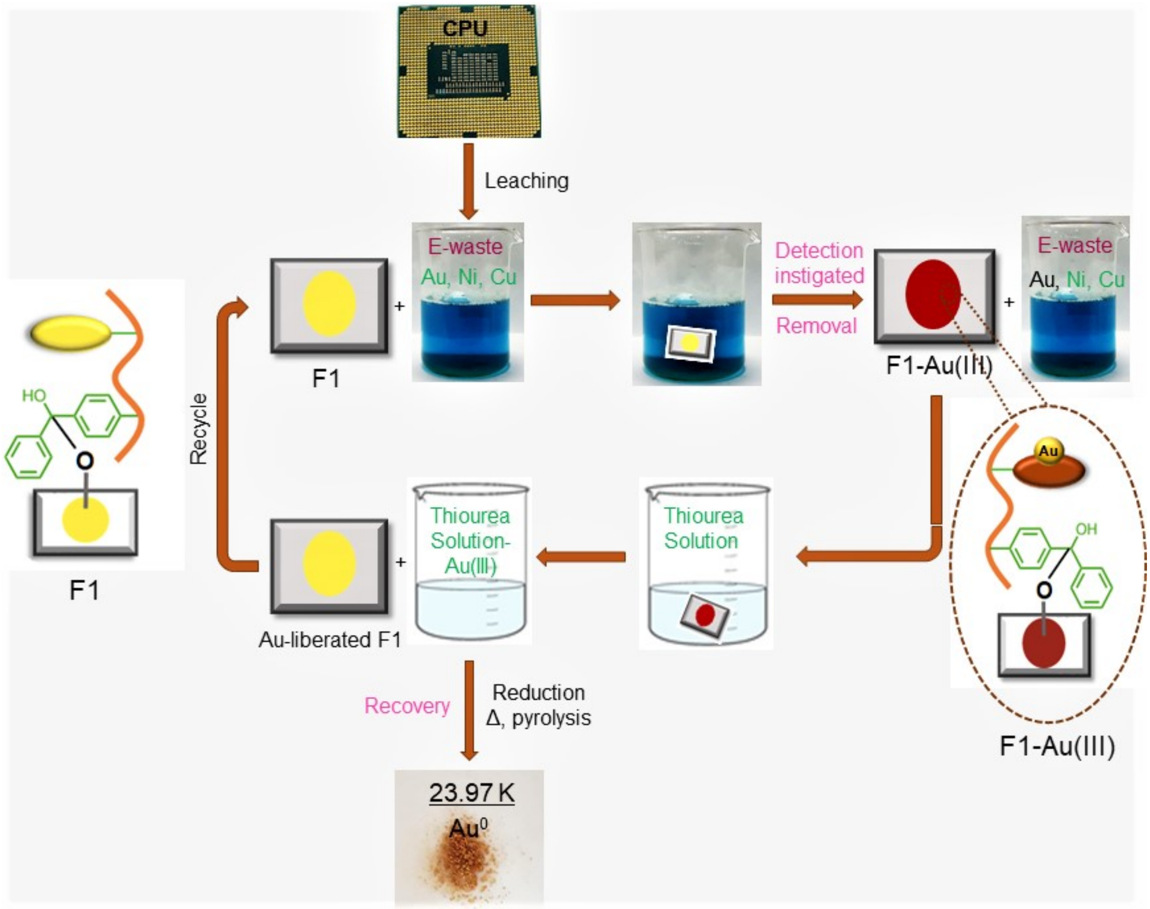
Chair: Jeung Gon Kim (Jeonbuk National University)

Gold recovery at ultra-high purity from electronic waste using selective polymeric film.

Rini Sharma, Hyung-il Lee[1,*]

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

Gold (Au) is extremely valuable in a variety of areas; however, its inadequacy increases the desire to recover it from any possible source, such as virgin mines and electronic waste (e-waste). Here we propose a sustainable Au recovery technology from e-waste with high purity and probe recyclability, which is established on selective 1:1 coordination-based colorimetric probes immobilized on the surface of a quartz substrate to form a thin polymeric film (F1). The presence of Au(III) in various e-waste samples was determined via the color changes from yellow to brick-red of F1, and this is used to decide if further Au recovery is lucrative. Thereafter, trace amounts of Au at ultra-high purity (23.97 K) are rapidly recovered (in 10 min) even with approximately 100-fold excess of other metal ions (copper and nickel) commonly found in e-waste without the use of harsh acids, bases, or toxic methods. Au(III)-liberated F1 can be used to further separate Au(III), and this process was repeated for multiple cycles.


CPU
Leaching
F1
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E-waste
Au, Ni, Cu
Detection
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Removal
F1-Au(III)
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Au-liberated F1
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Thiourea
Solution-
Au(III)
Thiourea
Solution
Recovery
Reduction
Δ, pyrolysis
23.97 K
Au⁰

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:24

Chair: Jeung Gon Kim (Jeonbuk National University)

Preparation and characterization of bio-based poly(L-lactide) gradient copolymer foams and their application to broadband sound absorption

Heeyoung Park, Seung-Yeop Kwak[*]

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

Recently, bio-based polymeric foams as sound absorbers have gained tremendous attention from the automobile industry for their low density, further reduced carbon emission, excellent sound absorption properties, etc. Despite these advantages, it still remains challenging to exhibit high sound absorption performance at lower frequency range caused by poor noise damping and tortuosity of foams. In this study, we present a facile method of fabricating bio-based poly(L-lactide-co-ε-decalactone) gradient copolymer foams (i.e., PLDL) for their application to broadband sound absorption. A series of PLDL copolymer foams were fabricated by ring-opening copolymerization of L-lactide and ε-decalactone monomers and subsequent thermally-induced phase separation with lyophilization. Our results demonstrate that the formation of bimodal nano-/micrometer pore structure increased foam tortuosity, eventually resulting in enhanced sound absorption at the low-to-mid frequency range. Besides, the incorporation of flexible ε-decalactone enabled the PLDL foam to show improved noise damping ability and reduced airflow resistivity and, thereby, induced enhancement of sound absorption coefficient in broad range of frequencies. As a result, excellent sound absorption performance of PLDL foams was achieved with higher sound absorption coefficient at lower frequency range and broadened bandwidth of sound absorption. These results may contribute to the ongoing efforts to produce environmentally sustainable sound absorption materials.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:36

Chair: Jeung Gon Kim (Jeonbuk National University)

Development of Smart Drug Delivery Platforms using Nanofibers

Baljinder Singh, Myoung-Hwan Park[1,*]

Department of Convergence Science, Sahmyook University, India
[1]*Department of Chemistry, Sahmyook University, Korea*

Smart drug delivery platforms using nanofibers are extensively applicable for customized drug release based on target location and timing to achieve the desired therapeutic effects. A nanofiber formulation is typically created for a certain medication and changing the drug may have a significant impact on the release kinetics from the same delivery system. Nanofibers have several distinguishing features and properties, including the ease with which they may be manufactured, the variety of materials appropriate for processing into fibers, a large surface area, and a complex pore structure. The gold nanorods (GNRs) present in nanofibers generate heat when exposed to near-infrared (NIR) radiation due to the plasmon resonance effect as the GNRs are absorbed in the range of the NIR spectrum. Upon NIR irradiation, the increase in temperature by GNRs make physical or chemical changes in nanofibers which ensured that the drug was released in a controlled manner. This research demonstrates a promising platform for safely delivering drugs and controlling drug release to treat cancer as well as other challenging diseases.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:48

Chair: Jeung Gon Kim (Jeonbuk National University)

Defect-free acrylic polymers with a near-Poisson distribution prepared via catalyst-free visible-light-driven radical polymerization

Changhoon Yu, **Min Sang Kwon**[1,*]

Materials Science and Engineering, Seoul National University, Korea
[1]*Department of Materials Science and Engineering, Seoul National University, Korea*

Reversible-deactivation radical polymerization (RDRP) based on direct photolysis has a favorable reaction structure for superior controllability compared to that of conventional RDRP. However, this aspect has not been fully demonstrated because the photolysis process is vaguely understood. In this study, we propose a mechanism for photolysis and apply the proposed mechanism to obtain polyacrylates with an extremely narrow dispersity approaching the Poisson distribution (an ideal molecular weight distribution attained in living polymerization) and a negligible fraction of dead chains (< 2%), even for very high conversion (> 90%) and short reaction time (5 h). Based on the results, extremely well-defined and defect-free α,ω-hydroxyl end-functionalized polyacrylates were prepared to utilize the resulting polyols as soft segments of thermoplastic polyurethane (TPU) elastomer. Using the prepared polyols, TPU elastomers that do not follow the conventional trade-off relationship of “strength−elongation” and “robustness−self healing ability” were successfully prepared, highlighting their potential as next-generation functional polymeric materials.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:00

Chair: Jeung Gon Kim (Jeonbuk National University)

Development of polymer based new platforms for in vitro study of neuronal cells

Thi Thuy Chau Nguyen, Sung Yun Yang[1,*], In Young Park[2]

Department of Polymer Science and Engineering, Chungnam National University, Vietnam
[1]*Department of Organic Materials Engineering, Chungnam National University, Korea*
[2]*Chungnam National University, Korea*

In order to study about cell behaviors in term of in vitro research, the development of biomaterial mimicking structure of extracellular matrix is very necessary. The studies of non-conventional cell culture system for stimulating cells have been received attention from researchers because of their controlled mechanical strength and high biocompatibility similar to biological tissues. In our research, we studied about the activities of neuronal cells cultured on the modified substrates of using polymer substrates and coatings specially designed as highly biocompatible. Various polymers as thin film coatings with micropatterns were developed, among them, the surfaces with spatially anisotropic alignment show significant effect on cell morphology and mobility. These interesting results indicated the role of the culture substrate in the responses and behaviors of neuronal cells, which bring the benefit to further in vitro studies and applications.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:12

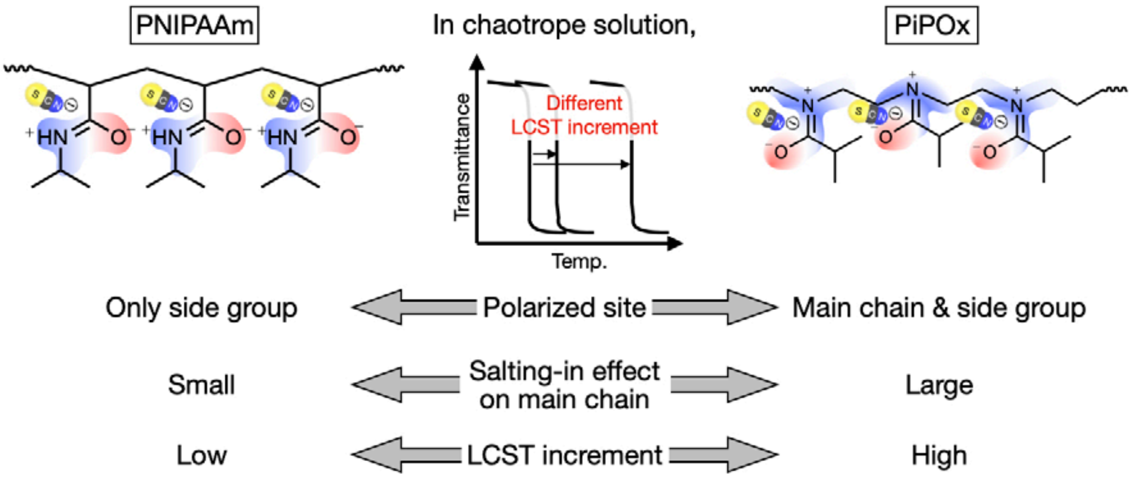
Chair: Jeung Gon Kim (Jeonbuk National University)

Effect of Anions on the Phase Transition Temperature of Two Structurally Isomeric Polymers: Poly(*N*-isopropylacrylamide) and Poly(2-isopropyl-2-oxazoline)

Taehun Chung, Jihoon Han[1], Younsoo Kim[*]

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

The effect of Hofmeister anions on the lower critical solution temperature (LCST) of two structural isomers, namely, poly(*N*-isopropylacrylamide) (PNIPAAm) and poly(2-isopropyl-2-oxazoline) (PiPOx), is studied. Following the preparation of these two polymers with the same molecular weights and chain ends, their thermal hysteresis and LCST properties are observed in the aqueous and Hofmeister salt solutions. We investigate the effects of the salt type and concentration on the LCST for both polymers. More specifically, the LCST of PiPOx sharply increases as the concentration of SCN^- increases, whereas that of PNIPAAm slightly increases prior to decreasing again. It is also confirmed that the boundary between the salting-out and salting-in effects is different for both polymers according to the type of salt present. Furthermore, Raman spectroscopy and two-dimensional correlation spectroscopy are used to examine the conformational changes of both polymers with increasing SCN^- (chaotropes) and Cl^- (kosmotropes) concentrations. Since the interaction mechanism between the polymer and anion is remarkably different even between isomeric polymers, it is necessary to rationally design the polymer structure to enhance the anion effect of the thermoresponsive polymer. This presentation will discuss the thermal hysteresis, changes of cloud point (T_{cp}), and the conformational changes of each polymer caused by the binding of anions.


PNIPAAm
In chaotrope solution,
PiPOx
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Transmittance
Temp.
Only side group
Polarized site
Main chain & side group
Small
Salting-in effect
on main chain
Large
Low
LCST increment
High

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:24

Chair: Jeung Gon Kim (Jeonbuk National University)

Large Area Freestanding Non-Metal Based Flexible Carbon Fiber Mesh for Water Electrolysis

Mohammad Boshir Ahmed, Myung-Han Yoon[1,*]

Materials Science & Engineering, Gwangju Institute of Science and Technology, Bangladesh

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

In this work, we report carbon fiber mesh (CFM) preparation from polyacrylonitrile and doped with sulfur. To do this, we prepared electrospun fiber mesh from a mixture of polyacrylonitrile and sulfur-based polymer at different compositions. Then electrospun fiber meshes were carbonized at 1000 oC in a programmable tube furnace to get CFMs. Finally, we have fabricated a binder and additives-free, highly porous freestanding CFM embedded with sulfur sites of exceptional activity and stability. Within the CFM, the sulfur atomic moieties exhibit higher conductivity and super wetting properties of the CFM promote electrolyte wetting and ensure the timely removal of evolving H2 gas bubbles. The as-designed CFM can work as an efficient non-metal-based HER electrode in acid. In addition, CFMs can be patterned into different forms. This finding paves the road toward the rational design of non-metal-based CFM with improved activity, paternity, super hydrophilicity, high conductivity, and stability in gas-evolving electrocatalytic processes.

Oral Presentation : **POLY.O-9**
Oral Presentation for Young Polymer Scientists
Room 303 THU 10:36
Chair: Jeung Gon Kim (Jeonbuk National University)

A Heavily Doped Doner-Doner Type Polymer with Metal-like Carrier Transport by Hybrid Doping

Changhwa Jung, Han Young Woo[1], Lee Hyunjung[*]

Materials Science & Engineering, Kookmin University, Korea
[1]Department of Chemistry, Korea University, Korea

Conjugated polymers (CPs) are suitable as thermoelectric (TE) materials for wearable devices due to their non-toxicity, flexibility, and low thermal conductivity. Despite the advantages of CPs as TE materials, CPs still have lower properties than other TE materials because of relatively low σ. Therefore, it is essential to improve the electrical conductivity (σ) and Seebeck coefficient (S) through the doping. Maintaining the crystallinity of CPs is significant to increase charge transport properties during the doping process. Dopants are effective when they penetrate both the crystalline and amorphous regions of the CPs. Various chemical doping methods have been proposed, including the solution-mixed doping method (MxD), sequential solution doping method (SqD), vapor deposition doping method, and dipping doping method. However, these doping methods collapse the crystallinity of the CPs or penetrate only the amorphous region. In this study, we used a hybrid doping method (HyD) to compensate for these shortcomings. We investigated the HyD effect through comparison with MxD and SqD. Also, we used donor-donor type Poly(4,9-bis(bis(hexylthio)methylene)-7-methyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophene-2-(4-(bis((2-hexyldecyl)thio)methylene)-6-methyl-4H-cyclopenta[2,1-b:3,4-b']dithiophen-2-yl)) which designed to have good charge transport properties and packing density. By comparing the Seebeck coefficient and electrical conductivity relation based on the Kang-Snyder charge transport model, we identified the variation of charge transport mechanism by different doping methods. Finally, our work provides strategies for TE materials showing high electrical conductivity through the optimized doping method.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:48

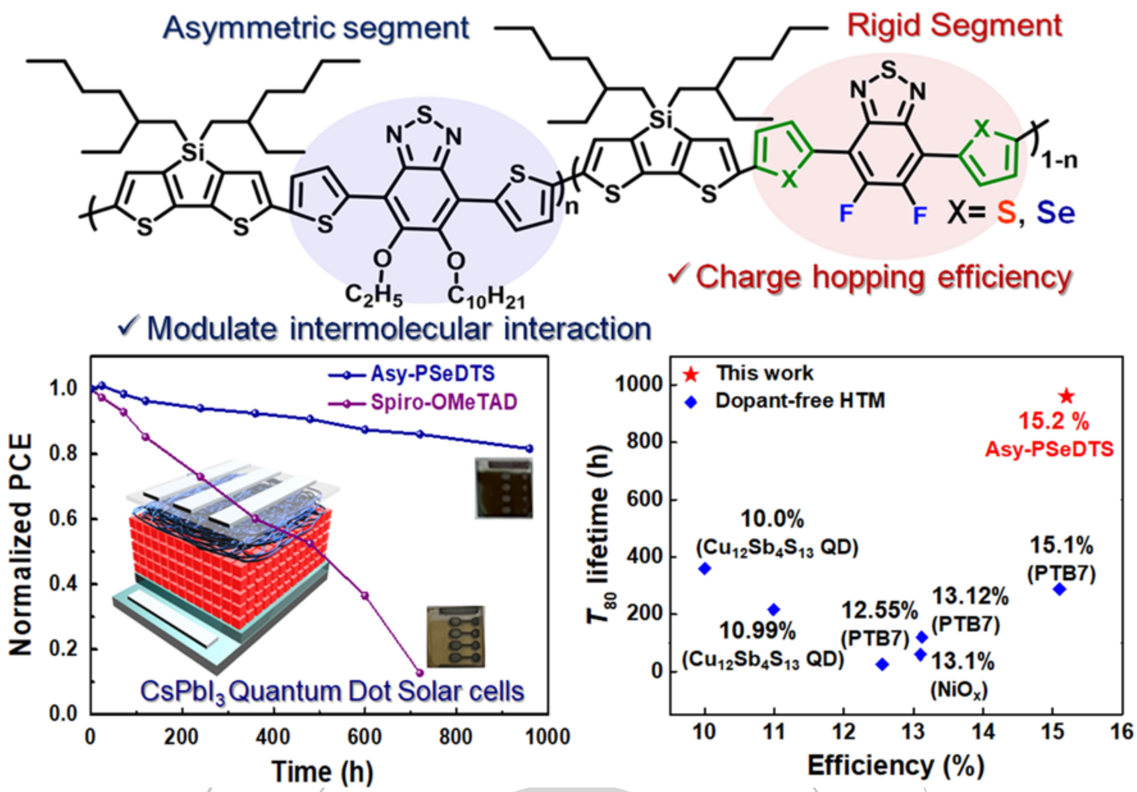
Chair: Jeung Gon Kim (Jeonbuk National University)

Tailored Novel Hole Transport Materials with Rigid Segments toward Efficient and Stable Perovskite Quantum Dot Solar Cells

Daehwan Lee, Seyeong Lim, Taiho Park*

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

CsPbI3 perovskite quantum dots (PQDs) with ideal optoelectronic properties offer high thermal stability for photovoltaics. However, PQDs are sensitive to external moisture or oxygen conditions and thus have poor phase stability. In this prospect, hydrophobic hole transport materials (HTM) on the PQD surface are crucial for achieving high device stability. Conjugated polymers with strong molecular packing have efficient charge transfer ability, but excessive intermolecular interactions degrade film-forming properties in perovskite, leading to interfacial non-radiative recombination. In this respect, side chain engineering (e.g. extended- and asymmetric chain, etc.) is developed for optimizing the morphological property. However, these strategies weaken the intermolecular interaction, reducing the efficiency of charge hopping. Herein, we proposed a new D-A conjugated polymer HTM design employing unsubstituted rigid segment. Interestingly, Asy-PSeDTS with rigid segment locally induces strong intermolecular interactions, enhancing the charge hopping efficiency. Thanks to these advantages, the Asy-PSeDTS-based PQD solar cells achieved 15.2% PCE and maintained 80% of the initial PCE after 1000 h, which is the highest PCE and stability among dopant-free HTM-based PQD solar cells.



Asymmetric segment
Rigid Segment
Si
S
N
O
C_2H_5
$C_{10}H_{21}$
n
1-n
F
X
X= S, Se
✓ Charge hopping efficiency
✓ Modulate intermolecular interaction
Asy-PSeDTS
Spiro-OMeTAD
Normalized PCE
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
1000
Time (h)
$CsPbI_3$ Quantum Dot Solar cells
This work
Dopant-free HTM
15.2 %
Asy-PSeDTS
10.0%
($Cu_{12}Sb_4S_{13}$ QD)
15.1%
(PTB7)
13.12%
(PTB7)
12.55%
(PTB7)
10.99%
($Cu_{12}Sb_4S_{13}$ QD)
13.1%
(NiO_X)
T_{80} lifetime (h)
1000
800
600
400
200
0
10
11
12
13
14
15
16
Efficiency (%)

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 09:00

Chair: Hongseok Yun (Hanyang University)

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

Chemistry, Chungbuk National 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. The TE material can be made using the Zintl phase, which is accessible to dope because it has a semiconductor property and a 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. Previous study shows 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 *p*-dopant to mix Cu^+ with Zn^{2+}, not only did the effect of Ca/Yb mixing, but the hole carrier concentration increased to obtain an overall synergy effect. A series of compounds in the $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ ($0.5\leq x\leq 4.5$; $0.05\leq y\leq 0.2$) system was synthesized using the conventional high-temperature method and the Pb-metal flux method, and we confirmed that the single-crystal with the bar-shaped grew nicely. Crystal structures were characterized by both powder X-ray diffractions and single-crystal X-ray diffractions. Theoretical calculations were also conducted through the tight-binding linear muffin-tin orbital method, and the DOS, COHP, and band structure of the three title compounds were analyzed to understand the electronic structure.

Oral Presentation : **INOR.O-2**
Oral Presentation for Young Inorganic Chemists
Room 407+408 THU 09:15
Chair: Hongseok Yun (Hanyang University)

Aliphatic and Aromatic C−H Bond Oxidation by High-Valent Manganese(IV)-Hydroxo Species

Yu jeong Lee, **Sunggi Lee**[1,*], **Jana Roithova**[2,*], **Jaeheung Cho**[*]

Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Korea
[1]*Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology (DGIST), Korea*
[2]*Institute for Molecules and Materials, Radboud University, Netherlands*

The strong C–H bond activation of hydrocarbons is a difficult reaction in environmental and biological chemistry. Herein, a high-valent manganese(IV)-hydroxo complex, $[Mn^{IV}(CHDAP\text{-}O)(OH)]^{2+}$ (2), was synthesized and characterized by various physicochemical measurements, such as ultraviolet–visible (UV–vis), electrospray ionization-mass spectrometry (ESI-MS), electron paramagnetic resonance (EPR), and helium-tagging infrared photodissociation (IRPD) methods. The one-electron reduction potential (E_{red}) of 2 was determined to be 0.93 V vs SCE by redox titration. 2 is formed via a transient green species assigned to a manganese(IV)-bis(hydroxo) complex, $[Mn^{IV}(CHDAP)(OH)_2]^{2+}$ (2´), which performs intramolecular aliphatic C–H bond activation. The kinetic isotope effect (KIE) value of 4.8 in the intramolecular oxidation was observed, which indicates that the C–H bond activation occurs via rate-determining hydrogen atom abstraction. Further, complex 2 can activate the C–H bonds of aromatic compounds, anthracene and its derivatives, under mild conditions. The KIE value of 1.0 was obtained in the oxidation of anthracene. The rate constant (k_{et}) of electron transfer (ET) from N,N´-dimethylaniline derivatives to 2 is fitted by Marcus theory of electron transfer to afford the reorganization energy of ET (λ = 1.59 eV). The driving force dependence of log k_{et} for oxidation of anthracene derivatives by 2 is well evaluated by Marcus theory of electron transfer. Detailed kinetic studies, including the KIE value and Marcus theory of outer-sphere electron transfer, imply that the mechanism of aromatic C–H bond hydroxylation by 2 proceeds via the rate-determining electron-transfer pathway.

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 09:30

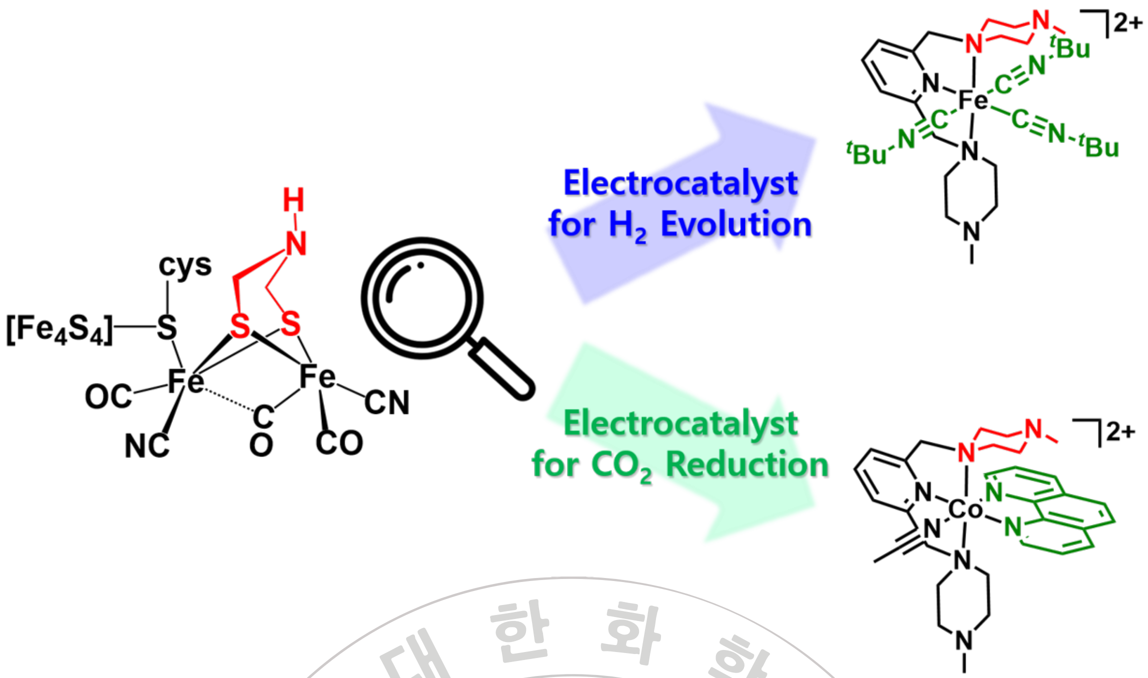
Chair: Hongseok Yun (Hanyang University)

Bioorganometallic Approaches in Electrocatalytic Reactions Using Structural Mimics of [FeFe]-hydrogenase

Seungjin Song, Junhyeok Seo*

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

Electrochemical reactions, such as the H_2 evolution reaction and the CO_2 reduction reaction, have been studied as alternatives to fossil fuels in the pursuit of sustainable energy systems. Developing electrocatalysts using bioorganometallic approaches has garnered attention due to the advantages of utilizing earth-abundant metal ions as catalysts and designing efficient catalysis inspired by the active site in the metalloenzyme. Specifically, we are interested in the active site of [FeFe]-hydrogenase, which contains dinuclear Fe ions and an azadithiolate ligand that bridges the two Fe ions. The nitrogen atom in the azadithiolate acts as a Lewis basic site, assisting in delivering protons to the Fe center and facilitating the H_2 metabolism of [FeFe]-hydrogenase. We synthesized NNN-pincer complexes with N-methylpiperazine arms as Lewis basic sites to mimic these functionalities. The N-methylpiperazine arms in our complexes successfully deliver the protons to the metal center and facilitate their electrochemical reactions. We also modulated the electronic properties of the metal center in NNN-pincer complexes using auxiliary ligands, such as the *tert*-butylisocyanide(^{t}BuNC) ligand and polypyridyl ligands, to control the electrochemical reactivity of the NNN-pincer complexes. Herein, we present the impact of the Lewis basic site on electrocatalytic reactions through a series of experiments and outline the methods for modulating the electrochemical reactivity of metal complexes.


H
N
cys
[Fe_4S_4]
S
S
S
OC
Fe
Fe
CN
NC
C
O
CO
Electrocatalyst for H_2 Evolution
Electrocatalyst for CO_2 Reduction
2+
^{t}Bu
N
C≡N
Fe
C≡N-^{t}Bu
^{t}Bu-N≡C
N
N
2+
N
Co
N
N

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 09:45

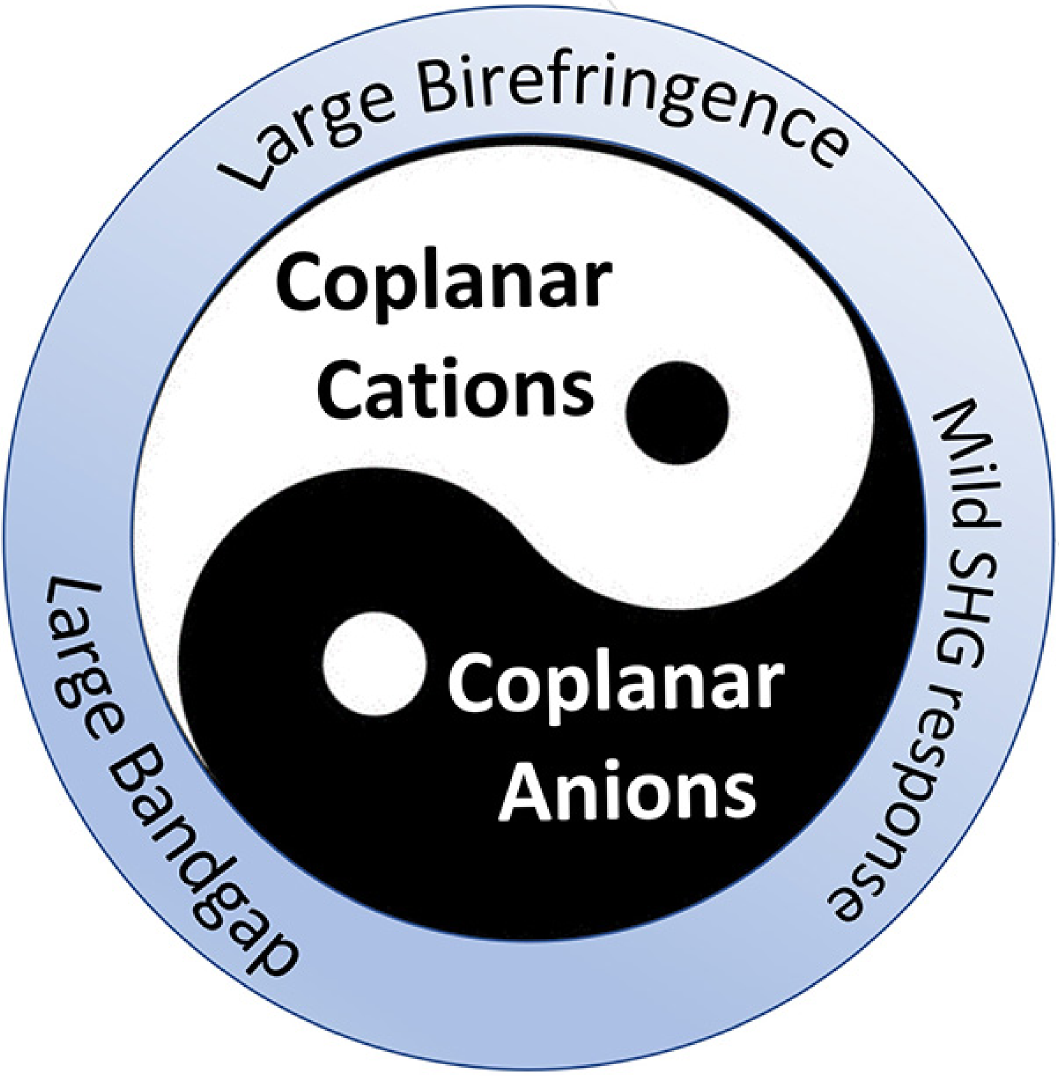
Chair: Hongseok Yun (Hanyang University)

Optical materials with giant birefringence and short UV cutoff edges

Yang Li, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Birefringent and nonlinear optical (NLO) materials are crucial components of laser-related and polarizing technology industries. Although commercial birefringent materials, such as α-BaB_2O_4 (α-BBO), $CaCO_3$, TiO_2, and YVO_4, can operate in the UV regions, they do not fulfill all the requirements. Coplanar groups, such as MO_3 groups (M = B, C, and N), six-membered rings (6-MRs) groups, possess large micropolarizability and are promising systems to explore new materials with large birefringence. Other factors, such as these birefringence-active groups' (BAGs) density and spatial distribution, also influence birefringence. However, enhancing the birefringence (~0.5 or even larger) while maintaining a large bandgap ($\geq$ 3.0 eV) remains a challenging task.In light of these factors, new birefringent materials, 4HPN, 4HPO, and 2APO were successfully designed by incorporating two different BAGs.This approach effectively maximizes the ρBAG and is achieved through the slow evaporation method. As expected, the nearly optimal arrangements of BAGs in these structures produce a giant birefringence.First-principles calculations reveal that they exhibit giant birefringence (0.496-0.563@532 nm), which is much larger than α-BBO (0.122@532 nm), $CaCO_3$ (0.171@633 nm), YVO_4 (0.225@633 nm), and TiO_2 (0.256@1530 nm).Furthermore, their experimental band gaps of 3.83-4.59 eV make them suitable for use in the UV regions. 4HPN also has a large second-harmonic generation response (~1.5 × KDP), making it a promising NLO material. Therefore, their large band gaps and giant birefringence make them excellent birefringent materials in the UV regions.


Large Birefringence
Coplanar
Cations
Mild SHG response
Coplanar
Anions
Large Bandgap

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 10:00

Chair: Hongseok Yun (Hanyang University)

Single-step chemical vapor deposition of edge-on oriented 2D conductive metal-organic framework thin films

Myeongggeun Choe, Hee Cheul Choi[1,*], Sarah Sunah Park[1,*], Ji Hoon Shim[1,*]

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

We demonstrated the synthesis of a conductive two-dimensional metal–organic framework (MOF) thin film by single-step all-vapor-phase chemical vapor deposition (CVD). The synthesized large-area thin film of $Cu_3(C_6O_6)_2$ has an edge-on-orientation with high crystallinity. $Cu_3(C_6O_6)_2$ thin film-based microdevices were fabricated by e-beam lithography and had an electrical conductivity of 92.95 S/cm. Synthesis of conductive MOF thin films by the all-vapor-phase CVD will enable fundamental studies of physical properties and may help to accomplish practical applications of conductive MOFs.

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 10:15

Chair: Hongseok Yun (Hanyang University)

Confinement Effect of Metal–Organic Frameworks on Electrocatalytic Hydrogen-Evolution Activity

Prabu Mani, Younghu Son[1], Minyoung Yoon[2,*]

Green-Nano Materials Research Center, Kyungpook National University, Korea
[1]*Department of Chemistry, Kyungpook National University, Korea*
[2]*Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea*

Owing to the growing energy demand, developing an active, stable, low-cost catalytic material for hydrogen production is necessary. In this context, cavity- or pore-directed chemical transformation is a promising approach to increase the catalyst stability and durability via pore confinement. Herein, we investigated the confinement effect of Zr-based metal–organic frameworks (MOFs) in the presence of a Ni-based molecular catalyst for the hydrogen evolution reaction (HER). To investigate this, we chose stable and porous Zr-based MOFs, NU-1000 (1) and MOF-808 (2), as host materials, and Ni-based square–planar complex (Ni-ATP, ATP = 2-aminothiophenolate) was used as an electrocatalyst (guest). The Ni-ATP complex was successfully incorporated inside the pores of MOFs 1 and 2, and the integrated materials [Ni-ATP@NU-1000 (1´), Ni-ATP@MOF-808 (2´)] were successfully characterized by various instrumental methods. The electrochemical results covey that, the integrated materials 1´ and 2´ show enhanced HER activity with significant improvement in their onset potential compared with their pristine MOFs. Owing to the pore confinement, the unstable Ni-ATP catalyst is stabilized by 1, leading to providing a higher HER activity with long-time durability in acid media. Overall, we demonstrated the improved catalyst stability, enhanced HER performance, and long-time durability of the model catalyst by protecting it through the confinement effect of MOFs.

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 10:30

Chair: Hongseok Yun (Hanyang University)

Functionalization of Metal-Organic Frameworks with Vinyl Group and Tetrazoles

Jooyeon Lee, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-Organic Frameworks (MOFs) are three-dimensional porous structures in which metal clusters and organic linkers are coordinatively connected. MOFs have great tunabilities on their structure along with ligands and metal clusters compared to other traditional porous materials such as active carbon. However, at the same time, their processability to practical applications are quite restricted due to their fragility from crystalline nature. Therefore, the physical mixture between MOFs and polymeric mixed matrix membranes (MMMs) have been extensively studied to overcome fragile characters.

Recently, we have successfully introduced vinyl group in MOFs, and demonstrated that the covalent connection between MOFs and MMMs through thiol-ene photo-polymerization.[1] In addition, we could introduced the secondary functional groups in the core part of MOFs through ligand exchange technique. In the following studies, the vinyl group in MOFs was utilized to assembly of MOFs and porous polymers at the surface of MOFs.[2]

In addition to carbon-based functional group, nitrogen-rich tetrazole was also successfully introduced in dicarboxylate ligand and MOFs.[3] The installed tetrazole groups showed enhanced proton conductivity and different mechanism from other acidic functional group in MOFs. These three studies clearly demonstrated the efficiency and utility of various organic functional groups in MOFs toward target applications and practical usages.

References

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2. N. Y. Ahn, J. Lee, W. Yeo, H. Park, J. Nam, M. Kim*, M. Seo*, *Inorg. Chem.* **2022**, *61*, 10365-10372.

3. D. Lee, S. Lee, Y. Son, J. Y. Kim, S. Cha, D. Kwak, J. Lee*, J. Kwak*, M. Yoon*, M. Kim*, *Bull. Kor. Chem. Soc.* **2022**, *43*, 912-917.

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

Oral Presentation for Young Inorganic Chemists

Room 407+408 THU 10:45

Chair: Hongseok Yun (Hanyang University)

Nanodiamond-based Thermometric Monitoring for the Detection of Mitochondrial Metabolism in Living cell

Yoobeen Lee, Jin Seok Lee[*]

Department of Chemistry, Hanyang University, Korea

Intracellular thermometry techniques provide information about biological activities. In particular, detecting temperature variations in targeted organelle under specific physiological conditions is of great help in understanding the thermogenesis dynamics of cells. However, reducing the size of biocompatible thermometers down to submicrometers and attaching them to organelles is a challenge. Here, we demonstrate the monitoring of the accompanying temperature change process in ATP generation inside living fibroblast cells by using mitochondria-targeting nanodiamond quantum thermometry based on nitrogen-vacancy color centers. We developed a microscopy system that incorporates a coplanar waveguide-integrated incubating chamber and a real-time particle tracking system for temperature monitoring of nanodiamonds moving within cells.Using this system, we measured temperature rise based on the thermogenic response of mitochondria by inhibiting of ATP synthesis. Our technique may allow for studying biological processes related to mitochondrial metabolism and interactions between mitochondria and other organelles.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:00

Chair: Junwoo Park (Sogang University)

Modeling of aqueous electrolyte solutions via machine learning for the development of rechargeable batteries for renewable energy storage

Yevhen Horbatenko, Minhaeng Cho, Stefan Ringe[*]

Department of Chemistry, Korea University, Korea

Rechargeable batteries have become indispensable for our daily life and are considered a promising technology for sustainable energy systems in the future. One of the most important parts of a battery is a liquid electrolyte which is critical in stabilizing the electrode−electrolyte interfaces and constructing safe and long-lifespan batteries. Both experimental and theoretical techniques were employed to study the structure of liquid electrolytes, however, they are limited. In particular, IR and Raman can only partially describe the structure, and ab initio calculations, e.g., DFT are limited due to computational cost and the sizes of models. To model a liquid electrolyte, we employ many-body expansion (MBE) which is an excellent common strategy to model large systems by partitioning energies into a hierarchy of decreasingly significant contributions (one-, two-, three-body, etc.), thus, allowing one to reduce the scaling problem of large systems. Moreover, for each term in the MBE decomposition, we employ machine learning techniques as an excellent alternative to reduce computational cost without loss of overall accuracy. As a model system for a liquid electrolyte, we use an aqueous solution of hydrochloric acid. Although still in the early stage, we will discuss the preliminary results of modeling the solution with H_2O (one-body), $(H_2O)_2$ (two-body), $(H_2O)_3$ (three-body) as well as $H^+(H_2O)$, and $Cl^-(H_2O)$. In the future, to reach a realistic description of the aqueous electrolyte, we will increase the degree of complexity by including additional species, such as $Cl^-(H_2O)_2$, $H^+(H_2O)_2$, as well as $H^+(H_2O)Cl^-$, $H^+(H_2O)_2Cl^-$, etc.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:10

Chair: Junwoo Park (Sogang University)

Investigating the Ion Transport Mechanism in Organic Ionic Plastic Crystals: the Effects of Point Vacancies and Grain Boundaries

Hyungshick Park, Bong June Sung[*]

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystals (OIPCs) are soft, yet crystalline solid electrolytes composed of organic ions. These ions can undergo rotational motions even in the crystalline phase at sufficiently high temperatures. OIPCs have a higher concentration of defects such as Schottky vacancy and/or grain boundary compared to simple ionic crystals. Defects, along with rotational motions, may facilitate the transport of dopant alkali ions, for which OIPCs are considered as a strong candidate for the solid electrolyte. However, current understanding of the ion transport mechanism at a molecular level with defects is limited. This might be due to the difficulty of controlling either type or concentration of defects systematically in experiments. In this work, we carry out atomistic molecular dynamics simulations for 1,3-dimethylimidazolium hexafluorophosphate ([MMIM][PF_6]) OIPCs with lithium ions doped. We find that both defects strongly facilitate the heterogeneous dynamics of $[MMIM]^+$ and $[PF_6]^-$ ions, but in different fashions. We also find that grain boundaries affect the gransport of Li^+ preferentially compared to the Schottky vacancies, resulting in higher Li^+ transference numbers at the grain boundary of [MMIM][PF_6].

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:20

Chair: Junwoo Park (Sogang University)

Accurate the spin-orbit coupling with a relativistic MRSF-TDDFT approach

Konstantin Komarov

Pohang University of Science and Technology, Korea

Relativistic MRSF-TDDFT is developed considering the spin-orbit coupling (SOC) within the mean-field approximation. The resulting SOC-MRSF faithfully reproduces the experiments with very high accuracy, which is also consistent with the values by four-component (4c) relativistic CASSCF and 4c-CASPT2 in the spin-orbit-energy splitting calculations of the C, Si, and Ge atoms. Even for the fifth-row element Sn, the SOC-MRSF yielded accurate splittings (～3 % error). In the SOC calculations of the molecular 4-thiothymine with a third-row element, SOC-MRSF values are in excellent agreement with those of SO-GMC-QDPT2 level, regardless of geometries and exchange-correlation functionals. The same SOC-MRSF predicted the anticipated chance of S_1 $(n\pi^*)$ → T_1 $(\pi\pi^*)$ intersystem crossing, even in thymine with only second-row elements. With its accuracy and practicality, thus, SOC-MRSF is a promising electronic structure protocol in challenging situations such as nonadiabatic molecular dynamics (NAMD) incorporating both internal conversions and intersystem crossings in large systems.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:30

Chair: Junwoo Park (Sogang University)

Open Quantum Platform: a novel framework for quantum chemistry software development

Vladimir Mironov

Chemistry, Kyungpook National University, Korea

Quantum chemistry is essential for understanding chemical and physical phenomena in substances and is becoming a routine tool in theoretical and experimental chemistry. The Open Quantum Platform (OQP) is a novel framework that simplifies quantum chemistry software development and increases its flexibility by decomposing quantum chemistry methods into building blocks with defined interfaces. OQP contains a set of high-performance primitives for quantum chemistry, including data manipulation, Gaussian basis set manipulation, one- and two-electron integrals, and convergence algorithms. It uses a generic implementation style for many of its algorithms, which allows for easy extension to novel quantum chemistry methods. With OQP, reference implementations for energy and gradient calculations in HF, DFT, and TD-DFT have been developed, which are readily available.OQP is distributed as a library with Python bindings for regular users and provides a sample Python program to run OQP as a usual quantum chemistry package. We also provide a powerful C-API interface for software developers to integrate OQP into their programs. OQP is designed to be open and flexible, allowing anyone to create and use their own quantum chemical primitive as long as it conforms to the interface standard. By enabling more efficient and flexible development of quantum chemistry methods, OQP is poised to accelerate progress in this field and facilitate new discoveries with far-reaching implications for chemistry and related areas.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:40

Chair: Junwoo Park (Sogang University)

Investigating the Impact of Spin Contamination on the Accuracy of UHF-DFT Calculations

Hayoung Yu, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Density Function Theory (DFT) is a powerful method for predicting the properties of chemical systems, but its accuracy can be limited by functional approximations and approximate self-consistent densities. To address this, the theory of density-corrected DFT (DC-DFT) has been developed, which defines two types of errors in DFT calculations: functional errors and density-driven errors. A practical HF-DFT method, which involves calculating the approximate functional on Hartree-Fock densities rather than self-consistent densities, has been shown to provide significant improvements by reducing density-driven errors. Based on HF-DFT, methods such as BL1p and HF-r^{2}SCAN-DC4 have been developed. However, for open-shell systems, unrestricted HF (UHF) calculations can suffer from spin contamination, leading to inaccurate results. In this study, we compare the results of open-shell HF-DFT calculations using spin-contaminated UHF densities to those obtained using a restricted open-shell HF scheme. Our findings reveal the limitations of spin-contaminated UHF densities and underscore the importance of accurate density treatment in DFT calculations.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 09:50

Chair: Junwoo Park (Sogang University)

Properties of DNA Catenanes: *in silico* Approach

Yeonho Song, Jun Soo Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Catenanes are mechanically interlocked molecules and have been used to build molecular machines, such as molecular switch and molecular motor, in the field of supramolecular chemistry. Here, we investigate the properties of catenanes that consist of small minicircles of double-strained deoxyribonucleic acids (dsDNA) using molecular dynamics (MD) simulations. Understanding of the mechanical bonding in DNA catenanes is highly desired to develop DNA-based molecular machines mimicking their counterpart in supramolecular chemistry. The distributions of distance and angle between two DNA minicircles reveal the basic properties of mechanical bonding in DNA catenanes. Rotational dynamics and time correlation functions between two DNA minicircles reveal their dynamics at the order of nanoseconds. This study provides an essential understanding of DNA catenanes for their applications.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 10:00

Chair: Junwoo Park (Sogang University)

Tau Protein Aggregation in Alzheimer's Disease: the role of Polyamine

Jinmin Lee, Sang Hak Lee*

Department of Chemistry, Pusan National University, Korea

Neurofibrillary tangles, which result from the aggregation of hyperphosphorylated tau proteins (p-tau), are a hallmark of Alzheimer's disease (AD). Despite extensive research, the molecular mechanisms underlying these abnormal aggregates remain poorly understood. One factor that may contribute to this is the strong electrostatic repulsion between p-tau proteins, which are highly negatively charged. We hypothesize that small charged molecules are necessary to compensate for this charge repulsion in making protein aggregates. Interestingly, free polyamine molecules exist in a polycationic form in the body, and previous research has shown that their concentration is significantly higher in the brains of AD patients than in normal brains. Therefore, we investigated the role of polyamines in inducing interactions between negatively charged proteins, using fluorescence microscopy. Our findings reveal that the presence of polyamines has a critical effect on tau protein aggregation. Moreover, we observed a synergistic effect on tau aggregation when divalent metal ions (Mg^{2+} and Zn^{2+}) were added. We also directly observed the transition from protein condensates to a filamentous morphology. These results shed new light on the mechanism of tau aggregation and represent an important step forward in developing treatments for Alzheimer's disease.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 10:10

Chair: Junwoo Park (Sogang University)

Panchromatic Fluorogenic Generation of Luminescent Silver Nanodots by Cluster Transfer

Eunhye Lee, Junhua Yu[1,*]

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

Silver nanodots with high expectations for biological and chemical applications are luminescent silver cluster cores protected with peptides, polymers, and ssDNA(single stranded DNA). Their photo-physical properties such as brightness or photo-stability greatly depend on protection groups. Spectrally pure silver nanodots are formed through process of silver cluster transference from PAA(polyacrylicacid) to ssDNA with the whole visible to near-IR regions. The advantages of transfer method compared to the direct generation of fluorophores are dramatic enhancement of emission intensity and excellent photo-stability. This transfer strategy also has great merits with fluorogenic spectral range and the speed up of fluorophore generation. Furthermore, we demonstrated surface silver cluster transference by micro-contact printing with PDMS stamps with visualizing multiple printed ssDNA on bright silver nanodots. These efforts can be applied for various fields including biological cellular staining and fluorophore printing.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 10:20

Chair: Junwoo Park (Sogang University)

Pulsed laser interference patterning transition metal carbides for stable total water splitting

Theerthagiri Jayaraman, Yewon Oh, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

The low-cost and efficient electrocatalysis is continuously pursued for the sustainable electrochemical energy conversion reactions. Among the non-noble metal catalysts, transition metal carbides (TMC) attract more interest due to their unique surface reactivity and catalytic properties resembling noble metals. In this study, we could able to synthesis a series of TMCs (Co_3C, Fe_3C, TiC, and MoC) materials via a facile pulsed laser ablation (PLA) technique in liquid medium without adding additional carbon sources. Acetone was used as solvent which also act as carbon source. Acetone solvent was decomposed by laser ablation beam and provide carbon atoms which could dissolve into the interstitial sites of transition metals by the high pressure and temperature generated via laser plasma plumes, resulting in the formation of metal carbides. The synthesized materials were characterized by XRD, TEM, Raman, FE-SEM and XPS. The electrocatalytic performance towards half-cell HER, OER and overall water splitting were systematically investigated. As a result, Co_3C exhibits an excellent OER performance while MoC high HER activity. The fabricated two electrode electrolyzer using MoC as both anode and cathode exhibited an excellent efficiency for the hydrogen fuel production when compared with other carbides. The present study demonstrates facile strategy in the preparation of TMC electrocatalysts for energy-saving efficient hydrogen fuel generation.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 10:30

Chair: Junwoo Park (Sogang University)

Change in molecular conductance induced by electron-molecular orbital interaction

YoungJu Park, Junwoo Park*

Department of Chemistry, Sogang University, Korea

We investigate the change in molecular conductance of a self-assembled monolayer (SAM) of alkanethiolates ($CH_3(CH_2)_{n-1}SH$, n=2, 4, 6, 8, 10, 12, 14, 16, 18) on a gold substrate with the applied bias voltage. We inject the electrons into the molecular orbitals by applying a bias voltage. As the applied bias voltage is higher than a threshold voltage, the electrons transit from the coherent tunneling regime to the incoherent tunneling regime (i.e., the electrons occupy the molecular orbital). In the incoherent tunneling regime, the electrons are accessible into the LUMO (lowest unoccupied molecular orbital) of the alkyl chain because the fermi level of the metal is higher than the LUMO of the alkyl chain, and a change in molecular conductance occurs. In the coherent tunneling regime, on the other hand, the electrons are not accessible into the LUMO, and there is no change in molecular conductance. Experimental results show that the correlation between the change in molecular conductance and the length of the alkyl chain of the alkanethiolates, and the change in molecular conductance increases with increasing chain length. We presume the electrons in the LUMO of the alkyl chain change the conformational structure of the alkanethiolates. Hence, this phenomenon could introduce a method to modulate the conductance of molecules which operate fast with a simple operation.

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

Oral Presentation for Young Physical Chemists

Room 401+402 THU 10:40

Chair: Junwoo Park (Sogang University)

Conformational study of heterocyclic compounds by IR resonant VUV-MATI mass spectroscopy

Sung Man Park, Chan Ho Kwon[*]

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

The conformational structure of a polyatomic molecule is essential for understanding chemical and biological activities. In particular, since the heterocyclic compounds such as morpholine (C_4H_9NO) and tetrahydrofuran (C_4H_8O, THF) are the basic building blocks for biological molecules, their conformational structures have been investigated by many physical chemists. However, their conformational stability still remains a subject of debate. We performed the conformational study of morpholine and THF using the recently developed IR resonant VUV-MATI mass spectroscopy. As a result, the conformational stabilities of the molecules could be determined by analyzing the identifiable vibrational spectra of individual conformers with the aid of the quantum chemical calculations. It revealed that for morpholine in the neutral ground state, the Chair-Eq conformer is more stable than the Chair-Ax conformer by $108 \pm 7\ cm^{-1}$. In the case of THF, it was concluded that the Twisted (C_2) conformer is more stable than the Bent (C_S) conformer by investigating the conformational preferences under various molecular beam conditions.

Oral Presentation : **PHYS.O-12**
Oral Presentation for Young Physical Chemists
Room 401+402 THU 10:50
Chair: Junwoo Park (Sogang University)

Complete Description of Second-Harmonic Generation in 2D Hetero-Structures by Polarization-Resolved Interferometry

Juseung Oh, Sunmin Ryu[1,*]

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

Second-harmonic generation (SHG) is a non-linear optical process that occurs when a non-centrosymmetric optical medium interacts with two photons of identical frequency to produce another photon with twice the frequency. Whereas SHG has been widely used to determine the crystallographic orientation of various 2D single crystals, its applicability to artificially stacked heterocrystals has not yet been established.[1] In this work,[2] we show that the SHG from hetero-bilayer transition metal dichalcogenides (TMDs) can be described as the vector sum of waves of SHG signals from each monolayer, which contains phase, amplitude, and polarization information. The new matrix representation of the vector sum enables a complete description of the SHG behavior from hetero-bilayer TMDs and reveals a fundamental relation between the phase and orientation that can be used to determine orientation. The phase and intensity were obtained by spectral phase interferometry for two orthogonally polarized components. For the MoS2/WS2 bilayer, which was produced by the dry transfer, it was confirmed that the phase changed continuously with respect to polarization, unlike in the monolayer case, and that its behavior could be predicted by the new matrix model. Furthermore, we demonstrated that the stack angle of the MoS2/WS2 bilayer could be determined from the polarized interferometric data using the relationship between the phase and orientation derived from the new model, which could also be operated in a raster-scanning mode for spatial mapping. The matrix method also enabled the acquisition of the phase difference between monolayers directly from the SHG polar plot of hetero-bilayer TMDs without the need for interferometry. This would facilitate phase measurement and could be a useful future direction of research.References[1] W. Kim, J. Y. Ahn, J. Oh, J. H. Shim and S. Ryu, “Second-Harmonic Young's Interference in Atom-Thin Heterocrystals”, Nano Lett. 20, 8825 (2020)[2] J. Oh, W. Kim, G.

Jeong and S. Ryu, “Complete Description of Second-Harmonic Generation in 2D Hetero-Structures by Polarization-Resolved Interferometry”, to be submitted (2023)

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:00

Chair: Je Hyun Bae (Chungnam National University)

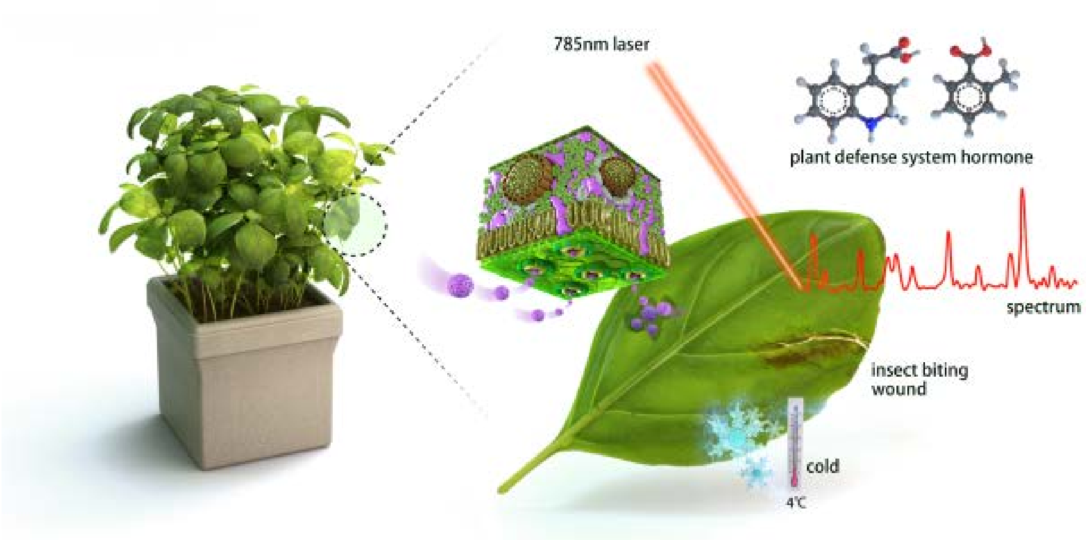
In vivo Real-time Multiplex Detection of Plant Signalling Molecules Using Surface-Enhanced Raman Scattering Nanosensor

WonKi Son, Dae Hong Jeong[1,*]

Department of Chemistry Education, Seoul National University, Korea

[1]*Department of Chemical Education, Seoul National University, Korea*

Recently, nanobiosensor technology has drawn interests in agriculture field due to its potential to overcome defects of existing materials as unique properties of nanomaterials. Nanobiosensor can provide information about plants into which nanobiosensor is introduced by detecting chemical signals of plants against various stressor such as fungal disease, water deficity and wound. Especially, spectroscopy using nanobiosensor has a few great advantages in that it is relatively invasive, cheap, simple analysis method that can identify chemcial structure. Raman spectroscopy, one of the spectroscopic methods, is suited to in vivo multiplex analysis due to narrow signal band width and no interference from water. Nonetherless, its weak signal intensity has been a major obstacle for application, but SERS spectroscopy that has dramatic signal enhancement on the surface of metal nanoparticles, has became a new alternative. In our research, we introduced PDDA-capped Ag bumpy nanoshell (PDDA@AgNS) into plants' leaf through stoma and detect SERS signal of plant hormones. First, we monitored real-time SERS signals from wound on leaf of watercress. Second, we also monitored SERS signals from leaves of barley/wheat that infected with fungal desease. In theses signals, we verified the multiplexity of PDDA@AgNS and further possibility of in situ and real-time monitoring of plant using nanobiosensors.


785nm laser
plant defense system hormone
spectrum
insect biting
wound
cold
4℃

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:04

Chair: Je Hyun Bae (Chungnam National University)

Lipidomic profiling on effects of intermittent diet in high fat diet-induced NASH mice using LC-MS

Yeajin Ju, Geum-Sook Hwang[*]

Korea Basic Science Institute, Korea

Altered lipid composition is one of the major reasons for nonalcoholic fatty liver disease (NAFLD). To date, no specific drug has been established, so intermittent fasting (IF) could be a new treatment strategy. Therefore, this study analyzes the therapeutic effect and underlying mechanism of intermittent fasting in NAFLD. In this study, C57BL/6J mice (male) were fed a normal diet (ND) and high-fat diet (HFD) and subjected to an alternated-day diet after 12 weeks for 35 weeks. Then, we performed global lipid profiling with liver from mice to estimate metabolic alteration using ultra-performance liquid chromatography/quadrupole time of fight mass spectroscopy (UPLC/Q TOF MS). Principal component analysis (PCA) score plots showed a separation between four groups in negative ion mode, however, there was only a difference in dietary effects in positive ion mode. We identified a total of 223 lipids. Most phosphatidylcholine was decreased in high-fat diet mice and showed a recovery pattern with intermittent fasting mice on high-fat diet mice. This study demonstrated that lipidomic profiling with LC-MS is a useful method to investigate the effects of intermittent fasting in obese mice.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:08

Chair: Je Hyun Bae (Chungnam National University)

A non-destructive Raman analysis of liver organoid and non-alcoholic fatty liver organoid (NASH)

Hoeil Chung[*], Sang hoon Cho[1]

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[1]*chemistry, Hanyang University, Korea*

In the past, animal testing was conducted on living animals with the aim of evaluating the possible negative effects on humans. However, the effectiveness of animal testing is rather controversial since symptoms appeared only in humans and ethical issue on animal testing is of a great concern nowadays. As an alternative, the use of organoids, cultured in human stem cells and have cell composition similar to actual organs, has been suggested. In this study, normal liver organoids (control groups) were cultivated and other organoids were also prepared as non-alcoholic fatty liver (NASH) with fatty acid, and Raman spectroscopy was employed for non-destructive measurement of the living organoids. The sizes of the organoids were tens of micrometers, and the entire organoids were measured at once in a specific conical-shaped container to amplify the Raman signal. Since NASH organoids were grown with various fatty acid concentrations, the uptakes of fatty acid were semi-quantitatively analyzed based on the acquired Raman spectra.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:12

Chair: Je Hyun Bae (Chungnam National University)

In-situ Spectroelectrochemical Analysis of Formamidinium Lead Iodide Perovskite Quantum Dots for Tracking their Degradation

Hyoin Kim, Taeyeon Kim[1], Seog Joon Yoon[2], Donghoon Han[*]

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

Multi-dimensional ABX3 hybrid perovskites have emerged as one of the key ingredients to be applied in many fields. Various forms of perovskites (dot, nanorod, platelet, bulk layer structure, etc.) are utilized by regulating the growth to depend on specific dimensions. Understanding the photoinduced charge carrier dynamics of perovskite quantum dots (PQDs) under electrochemical reactions can be a significant factor in applying perovskite quantum dots to solar-driven chemistry and optoelectronic devices. In this study, the reaction products were identified through cyclic voltammetry, X-ray photoemission spectroscopy, in-situ UV/Vis absorption spectroscopy, and detailed conversion reaction mechanisms of lead iodide perovskite quantum dot form were studied under electrochemical reactions. Comprehensive characterization identified irreversible oxidation transformation mechanisms for PQDs. This study can provide deep insight into the electrochemical behavior of PQDs for the successful application of solar-driven chemistry and optoelectronic devices.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:16

Chair: Je Hyun Bae (Chungnam National University)

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

Seunghee Shin, Myeong Hee Moon[*]

Department of Chemistry, Yonsei University, Korea

Human skin functions as a primary physical barrier against the external environment. The main constituents of stratum corneum, the outermost layer of epidermis, are lipids such as ceramides and glycerolipids. Tape stripping is one of the most efficient skin sampling method. 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 was focused to optimize skin sampling method in terms of sampling location and the number of tape strips in case of repeated stripping. Skin samples from ten sequential tape strips from the same spot and those from five sequential tape strips from 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. As the skin samples were taken from a same location repeatedly, the amount of identified lipid species had a tendency to decrease along with the slight variations in lipid composition, and it was largely decreased 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. More than 100 lipid species were in addition identified from pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strip for sample pooling, variation in lipid composition and amounts among the adjacent spots was evaluated in advance. 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. Sample pooling was adopted to establish the most representative tape stripping method that can represent skin lipid composition and avoid loss of any other quantifiable lipids.


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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:20

Chair: Je Hyun Bae (Chungnam National University)

Tuning Plasmonic Properties by Thiol in 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*

Mesoporous Silica Coated Gold Nanorods (AuNR@mSiO_2) was investigated with mercury amalgam and thiolation to study the plasmon effect of the AuNR@mSiO_2 during the reaction with mercury and thiol AuNR@mSiO2. In this work, we first incubation nanoparticles using mercury and LSPR peak of single-particle was study using dark-field microscopy and spectroscopy. Then, LSPR peak of the AuNR@mSiO_2 showing blue shifting and broadening in the linewidth as present from previous study. Interestingly, the peak was going to red shifting after the solution was changed into thiol and narrowing in they LSPR. To check the influence of the thiol, variant carbon length was using for this study. The peak become narrower due to the increase of the carbon length. This condition giving promising study to study the plasmon behavior of the AuNR@mSiO_2 and can be using for many applications, such as drug delivery and sensor.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:24

Chair: Je Hyun Bae (Chungnam National University)

An Image-Based Deep Learning Approach for Predicting Essential Mechanical Properties of Hydrogels

Jumi Kang, Kyueui Lee*

Department of Chemistry, Kyungpook National University, Korea

Hydrogels have significant potential as scaffolds in tissue engineering, and their mechanical properties, such as modulus and viscosity, must be tailored to the intended application. Therefore, predicting the mechanical properties is critical for developing effective hydrogel-based biomaterials. However, conventional mechanical testers like rheometers are costly, time-consuming, and require expertise in rheology. To address this challenge, we developed an image-based deep learning model that can predict essential mechanical properties, including viscosity, density, rigidity, and porosity, of hydrogels by simply analyzing SEM images. Specifically, we applied a Convolutional Neural Network (CNN) to extract relevant features from the input data and used an unsupervised method called Variational Autoencoder (VAE). This approach has two key characteristics: it learns the data distribution to recognize image group characteristics and generates new data based on the reconstructed image to differentiate between two groups: non-porous and porous structures. Our neural network model can help to reduce the time and cost associated with analyzing the mechanical properties of hydrogels in the short term. Moreover, given the ease of data production, our approach may reveal previously unknown mechanical characteristics of hydrogels, opening up new opportunities for tissue engineering and biomaterials development.

Oral Presentation : **ANAL1.O-8**
Oral Presentation of Young Analytical Chemists Ⅰ
Room 301 THU 09:28
Chair: Je Hyun Bae (Chungnam National University)

Lipidomic analysis of mice brain and spleen with SARS-CoV-2

Hwangyu Park, Myeong Hee Moon[1,*]

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

SARS-CoV-2 (severe acute respiratory syndrome coronavirus) has caused pandemic in the past three years. While most people recover from the disease except few severe illness, there are a number of people suffered from loss of taste or smell, fatigue, headache, muscle aches, and diarrhea besides respiratory symptoms. Moreover, although there are many evidences that viral infection occurs in various tissue other than lungs, lipidomic analysis has rarely been conducted so far except for blood, plasma, or serum.Lipids are not only used as energy sources and cellular components, but are also involved in signal transduction and permeability of cell membranes. Due to these various role of lipids, viral infection is expected to induce significant alternations in lipids in metabolic pathway.For investigate lipid perturbation by the SARS-CoV-2, qualitative and quantitative analysis have been performed in the brain and spleen tissues of transgenic mice expressing the human angiotensin converting enzyme 2 driven by the k18 promoter. In this study, brain and spleen samples were obtained from mice groups at six different time points (1, 2, 5, 7, 10, and 14DPI (day post infection) with two different plague forming unit (PFU) along with control and their lipid profiles were examined using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS).As a result of qualitative analysis, a total of 593 and 926 lipids were identified from the brain and spleen samples, respectively. Compared to the brain acyl chains of TG and phospholipid were more diverse in spleen. From targeted quantification, LPC, known to be associated with inflammation showed a decrease during infected periods, but PC showed an increase with the increase of PFU. Quantitative analysis of other lipid classes at the molecular level is still on going and their results will be introduced.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:32

Chair: Je Hyun Bae (Chungnam National University)

Dielectrophoretic Control of Plasmonic Metal Nanoparticle onto The Patterned Substrate for SERS-Active Substrate

Yun Su Yeo, Seunghyun Lee[1,*]

Department of Applied Chemistry, Hanyang University, Korea

[1]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*

Dielectrophoresis (DEP) induces dipoles to cause movement of particles. When a polarizable particle is placed in a non-uniform electric field, a dipole is induced due to the non-uniform electric field, resulting in a force imbalance at both ends. In DEP, it is essential to generate an electric field gradient, and the method mainly used is to fabricate a unique type of electrode. We will fabricate a SERS active substrate with uniformly arranged particles by applying DEP to plasmonic metal nanoparticles. Plasmonic metal nanoparticles have a unique phenomenon called LSPR, which is caused by the collective oscillation of electrons on the surface, and SERS arises from this phenomenon. Since LSPR occurs more strongly in a nanogap called a hotspot between nanoparticles and a metal structure, it is important to generate many hotspots to induce the SERS effect. In addition, since a uniform structure with a uniform nanogap is required, the particles must be uniformly arranged. However, it is very difficult to arrange the nanoparticles uniformly. Therefore, we will fabricate a SERS active substrate for molecular detection by inducing particle motion using DEP and arranging them to have a constant nanogap.In this study, gold-coated silica nanoparticles and patterned silicon substrates are used. The silicon substrate has regularly arranged circular patterns and is coated with a thin gold film due to the low conductivity of silicon. In DEP, particles having a diameter of about 800 nm were used because the larger the volume of the particle, the more sensitive it is to DEP. And it was confirmed that a relatively strong electric field gradient was formed at the edge of the cylindrical pattern through FDTD simulation (COMSOL Multiphysics, AC/DC Module).

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:36

Chair: Je Hyun Bae (Chungnam National University)

A simple strategy to improve SERS detection sensitivity in a small volume well-plate

Jiadong Chen, Jaebum Choo[1,*]

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

Surface-enhanced Raman scattering (SERS)-based sandwich immunoassay has been used to analyze target antigens using antigen-antibody interaction quantitatively. Capture antibodies are immobilized on the two-dimensional surface of a 96 well-plate, and then target antigens and SERS nanotag-labeled antibodies are sequentially combined to form sandwich immunocomplexes. One could perform the quantitative analysis of a target antigen by monitoring the characteristic Raman peak intensity of the SERS nanotag after creating sandwich immunocomplexes. However, immunocomplexes formed on a two-dimensional surface have a limitation in loading density due to a limited surface-to-volume ratio, resulting in poor sensitivity. In addition, when using a 96-well plate, a large sample volume is required for one well, and there is a limit to high throughput assay. To resolve these problems, we developed a highly sensitive SERS-based assay platform using SiO2 microparticles and a 1536-well plate. It was possible to improve the detection sensitivity of a target by increasing the surface-to-volume ratio with three-dimensional SiO2 microparticles. When performing the SARS-CoV-2 assay using the proposed platform, the detection limit could be improved more than ten times compared to the assay result using a 96-well plate-based absorbance enzyme-linked immunosorbent assay (ELISA).

A simple strategy to improve SERS detection sensitivity in a small volume well-plate

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Surface-enhanced Raman scattering (SERS)-based sandwich immunoassay has been used to analyze target antigens using antigen-antibody interaction quantitatively. Capture antibodies are immobilized on the two-dimensional surface of a 96 well-plate, and then target antigens and SERS nanotag-labeled antibodies are sequentially combined to form sandwich immunocomplexes. One could perform the quantitative analysis of a target antigen by monitoring the characteristic Raman peak intensity of the SERS nanotag after creating sandwich immunocomplexes. However, immunocomplexes formed on a two-dimensional surface have a limitation in loading density due to a limited surface-to-volume ratio, resulting in poor sensitivity. In addition, when using a 96-well plate, a large sample volume is required for one well, and there is a limit to high throughput assay. To resolve these problems, we developed a highly sensitive SERS-based assay platform using SiO_2 microparticles and a 1536-well plate. It was possible to improve the detection sensitivity of a target by increasing the surface-to-volume ratio with three-dimensional SiO_2 microparticles. When performing the SARS-CoV-2 assay using the proposed platform, the detection limit could be improved more than ten times compared to the assay result using a 96-well plate-based absorbance enzyme-linked immunosorbent assay (ELISA).

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:40

Chair: Je Hyun Bae (Chungnam National University)

Induced Electrospray Ionization Mass Spectrometry for the Analysis of Metabolites and Proteins at a Single Cell Level

Hyunsoo Kim, Sangwon Cha*

Department of Chemistry, Dongguk University, Korea

Conventional electrospray ionization (ESI) has been a workhorse for the mass spectrometric analysis of both small molecules like metabolites and biomacromolecules like proteins. However, conventional ESI often suffers from unstable and inefficient spray with a salt-containing sample and undesirable oxidation. In this study, we constructed an induced ESI(InESI) source to partially overcome these issues and investigated the applicability in the analysis of metabolites and proteins at a single cell level. In InESI, alternating current(AC) high voltage(HV) is applied to a sample solution in a non-contacting manner, while direct current(DC) HV is applied by directly contacting an electrode to a sample solution in conventional ESI. With InESI, proteins were found to be less oxidized and form less salt-adduct ions than conventional ESI. Furthermore, InESI enabled more efficient and stable ionization with an extremely small volume(~picoliter) of sample solution than conventional ESI. These features of InESI could ensure highly sensitive analysis with a trace amount of sample solution and thus could be highly beneficial in cell metabolite or protein analysis at a single cell level. Therefore, we tried to obtain single cell ingredients with a microscope-aided cell manipulation system and perform direct analysis of the obtained cell fluid by InESI mass spectrometry(MS). Our results suggest that InESI MS could serve as a highly sensitive and reproducible single cell MS platform.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:44

Chair: Je Hyun Bae (Chungnam National University)

Development of Sample Preparation Methods for Liquid Chromatography Tandem Mass Spectrometric Analysis of Ingredients in Household Chemical Products

Hyeonjeon Cha, Tae-Young Kim[1,*], Woo Young Song[2]

Gwangju Institute of Science and Technology, Korea

[1]*School of Earth Sciences and Environmental Enginee, Gwangju Institute of Science and Technology, Korea*

[2]*Earth Sciences & Environmental Engineering, Gwangju Institute of Science and Technology, Korea*

Recently, there has been increased concern regarding exposure to unknown hazardous chemicals in household chemical products (HCPs). However, there is a limitation to identify unrevealed ingredients in HCPs with a single analytical method due to their diverse physicochemical properties. Suspect screening analysis using liquid chromatography–mass spectrometry (LC-MS) is an effective technique to identify polar compound in HCPs. In this study, we developed a sample preparation method for HCPs and identified uncovered ingredients in the products.The following three types of HCPs were selected for the present study according to the product formulation: aerosol, water-soluble liquid, and water-soluble powder type. Basic condition solid phase extraction (SPE) using 0.02% ammonium hydroxide solution was performed to remove anionic surfactants in HCPs. Extracted samples were analyzed using a UHPLC-Q-TOF mass spectrometer, and chemicals were identified using NIST 20 MS/MS spectral library. As a result, fatty acids showed decreased intensity in the basic condition SPE compared to acidic SPE. Suspect screening analysis revealed unknown seven compounds across the tested HCPs, which were matched against commercially available reference standards. For the confirmed chemicals, recovery tests were performed using matrix matched calibration methods.The developed sample preparation method can provide knowledge of unknown hazardous chemicals in HCPs.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:48

Chair: Je Hyun Bae (Chungnam National University)

Lipidomic analysis in aorta tissue from ApoE knockout mice model of diabetes induced atherosclerosis using LC/MS

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

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

Atherosclerosis is the leading cause of most cardiovascular diseases, and diabetes is known to accelerate the progression of atherosclerosis. However, the mechanism of diabetes-accelerated atherosclerosis is still not fully understood. In the present study, we investigated the alteration in lipid metabolism related to diabetes in atherosclerosis using liquid chromatography tandem mass spectrometry (LC/MSMS).5-week-old ApoE knockout mice were designed three groups: normal diet (ND) group fed a normal diet, high fat diet (HFD) group fed a high fat diet, and streptozotocin (STZ) group fed a high fat diet and injected with STZ. Aorta tissues were obtained by sacrificing 10-week-old and 12-week-old mice.Partial least squares-discriminant analysis (PLS-DA) score plots showed a clear separation between HFD and STZ groups compared to the ND group in positive and negative modes, respectively. A total of 228 lipid metabolites were identified in aorta tissues. Especially, phosphatidylglycerols (PGs) and triacylglycerols (TAGs) were significantly changed in the HFD group compared to the STZ group. PGs were observed to promote atherosclerosis in diabetes by a specific chain at 12 weeks and TAGs were confirmed to have a unique pattern according to chain length and presence of diabetes.Our finding suggested that PGs might accelerate atherosclerosis in diabetes and demonstrated that lipidomic profiling using LC/MSMS is useful for understanding aorta lipid metabolism in diabetes induced atherosclerosis mice.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:52

Chair: Je Hyun Bae (Chungnam National University)

SERS-based SARS-CoV-2 assays using gold nanoparticles-encoded M13 bacteriophage networks

Joung-Il Moon, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

We developed a new SERS-based assay platform that can detect severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) with high sensitivity. First, we assembled M13 bacteriophage networks by controlling the concentration of M13 bacteriophage solution. Then gold nanoparticles (AuNPs) synthesized by the citrate reducing method attached to pVIII surface capsid proteins on M13 bacteriophage using thiol-PEG-NHS chemical linker. Finally, AuNPs-encoded M13 bacteriophage networks were deposited on the silicon wafer. When this substrate is exposed to laser light, the incident field is dramatically enhanced at active sites known as electromagnetic “hot junctions” generated by narrow nanogaps between AuNPs on the surface of M13 bacteriophage networks. In this study, a nuclear protein antibody was used as a receptor, and the AuNPs-embedded M13 bacteriophage network was used as a SERS substrate for the sensible detection of SARS-CoV-2. A quantitative analysis of SARS-CoV-2 lysate was performed by monitoring the change in the SERS peak intensity caused by the formation of sandwich immunocomplexes binding between the antibody-conjugated SERS nanotags and the SARS-CoV-2 virion. The results in this study demonstrate the possibility of a clinical application of this SERS-based assay platform that can dramatically improve the detection limit and accuracy of the currently commercialized SARS-CoV-2 assay kits.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 09:56

Chair: Je Hyun Bae (Chungnam National University)

Analysis and Differentiation of Citronella Oil by Gas Chromatography and Paper Spray Ionization Mass Spectrometry

Sumin Kang, Sangwon Cha*

Department of Chemistry, Dongguk University, Korea

Citronella oil is an essential oil obtained from the leaves and stems of Cymbopogon and has been used widely as a source of scent chemicals in various products such as soap, candles, and incense. Citronella oil also has been known to act as an insect repellent. There are two representative types of citronella oils, Java and Ceylon types, and their constituents and contents are listed in the international organization for standardization(ISO). Chemical analysis of citronella 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 an alternative and fast chemical fingerprinting method by using paper spray ionization MS (PSI MS). PSI utilizes a triangular paper tip for sampling and ionization and enables direct liquid sample analysis with minimal sample preparation. For sensitive detection of functional ingredients of citronella oil including citronellal, citronellol, and geraniol, the parameters for PSI such as spraying solvent composition, spraying voltage, and paper substrate were carefully optimized. We obtained chemical fingerprints from several citronella oil products of two different types by using GC-FID, GC-MS, and optimized PSI MS. Then, chemical fingerprint data obtained from three different analytical platforms were subjected to principal component analysis (PCA) for evaluating the performance of type-differentiation. Through this investigation, we found that PSI MS can serve as a quick and effective tool for differentiating citronella oil products.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:00

Chair: Je Hyun Bae (Chungnam National University)

Trends of PSA proteomes between prostate cancer tissues and blood among 20 cancer patients for early diagnosis

Miseon Jeong, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Korea

Prostate-specific antigen (PSA) is a protein biomarker isolated from the prostate tissue to blood and has been used to screen for prostate cancer (PCa). PSA tests in the blood could raise many false positive diagnoses and then induce follow-up tests such as biopsies which may be unnecessary and potentially dangerous. This study intended to discover the relationship between blood tests in clinics and cancer tissues by determining the PSA ranks in tissue proteomes of PCa patients with different PSA values in their blood for more accurate early diagnosis. The PCa tissues were collected from twenty PCa patients with different PSA values in blood tests. All PCa tissues were homogenized, and proteins were extracted with lysis buffer but detergent. Then each supernatant fluid was trypsin digested and desalted. The proteomes in all PCa tissues were identified and quantified using nLC-MS/MS and protein database search software. The protein ranks in each PCa tissue, including PSA, were determined based on the number of peptides with high confidence levels and protein scores. Then the PSA rank in cancer tissue was compared with the PSA value in each PCa patient's blood according to clinical information.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:04

Chair: Je Hyun Bae (Chungnam National University)

Fabrication of Mesoscopic Star-Shaped Gold Particles as SERS-active Substrate

Sumin Kim, Sunghoon Yoo, Seunghyun Lee[1,*]

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SERS(Surface-enhanced Raman Spectroscopy) is a highly sensitive molecular detection technique that enhances Raman scattering of molecules adsorbed on metal nanoparticles or nanostructures. Recently, major efforts have been made to synthesize precious metal nanoparticles of various sizes and shapes, which can control surface plasma resonance (LSPR). Complex geometrical structures with numerous sharp projections show LSPR scattering peaks at multiple wavelengths of direction and polarization. In gold meso-star synthesis, a three-step seed-mediated chemical method can give a high-yield synthesis of gold meso-star. Without silver nitrate, irregular and uncontrollable shapes of gold particles are formed. But when silver nitrate is added at the end, we can synthesize star-shaped gold microparticles with numerous sharp tips on their surface due to silver ions' effect on multi-directional growth, and they can generate strong local field enhancement. The more hot spots are formed by the Localized Surface Plasmon and the larger the particle size, the SERS signal increases. Gold meso-stars have strengths in both factors, so they can be used in various fields such as bio-molecular sensing. We have arranged gold meso-star particles to patterned substrates and then investigated whether they can be used as a highly sensitive SERS-active substrate.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:08

Chair: Je Hyun Bae (Chungnam National University)

Investigation of C-N Bond Formation in Microdroplet Formed by Electrospray Ionization–Mass Spectrometry

Byeongho Kwak, Sangwon Cha[*]

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The increasing concentration of carbon dioxide (CO2) in the atmosphere has led to serious environmental issues, making the investigation of carbon dioxide utilization crucial. In this study, we investigated carbon-nitrogen(C-N) bond formation between CO2 and amine compounds in microdroplets as a possible way of carbon dioxide utilization. Reactions in microdroplets have been known to be accelerated due to the surface area to volume ratio increase, the partial solvation, the reagent confinement effect, or the extreme pH condition. In order to realize microdroplet chemistry with CO2, we utilized electrospray ionization (ESI) as a reaction platform and resulting products were monitored in real-time by mass spectrometry (MS). Several methods for direct CO2 introduction into a solution have been tried such as utilization of carbonated water and addition of carbonate/bicarbonate salts into a solution. In addition, since the reaction acceleration in the microdroplet is thought to be often associated with the gas-liquid interfacial environment, we utilized CO2 nebulization gas or dry ice to ensure that the ambient condition surrounding the microdroplets are rich in CO2. We evaluated various CO2-introduction strategies by monitoring production yield of carbamic acids, expecting C-N bond formation products, and tried to determine the critical factors that accomplish accelerated C-N bond formation between CO2 and amine compounds.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:12

Chair: Je Hyun Bae (Chungnam National University)

Alginate Characterization Strategy through Absolute Monosaccharides Quantification utilizing PMP Labeling and LC/MRM-MS

<u>Hong Ju Kim</u>, Hyun Joo An[1,*]

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Alginic acid, which is widely used in various industries such as food, biomedicine, and pharmaceuticals, is a polysaccharide derived from cell walls of brown algae. Alginate is composed of randomly arranged hexuronic acid residues β-D-mannuronic acid(M) and α-L-guluronic acid(G) with 1,4-glycosidic linkages. Recently, it has attracted attention as a new functional biomaterial as it has been found to exhibit various biological activities such as antioxidant, antitumor, and immunomodulatory. Nevertheless, elucidating the relationship between structural properties and biological function remains challenging due to the lack of tools to characterize alginate. Here, we introduce an alginate characterization strategy through simultaneous absolute quantification of 14monosaccharides commonly found in nature based on LC/MRM-MS. Monosaccharides with isomeric structures were baseline separated and monitored via PMP labeling and structure-specific ions produced by MS/MS. This method allowed us to obtain the most important information about alginate: the ratio and purity (i.e. content) of M and G. In fact, 14monosaccharides could be successfully absolute quantified from attomole to femtomole in alginate extracted from seven species, which are brown algae in Korea. As a result, we determined that the extracts derived from various brown algae contained more than 60% of alginate, among which M/G ratio was 1.7 for Ecklonia cava and 2.5 for Ishige okamurae. Ultimately, our analytical platform and results will serve as a useful reference for understanding the structure and properties of alginate.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:16

Chair: Je Hyun Bae (Chungnam National University)

Development of 3D heterostructured MOF-derived B-doped Cobalt/Cobalt-oxide@N-doped carbon for effective alkaline water-splitting activity

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The sluggish oxygen evolution reaction (OER) at the anode and hydrogen evolution reaction (HER) at the cathode in alkaline media demands high overpotentials for water-splitting which require high-cost catalysts like Pt and IrO2/RuO2, etc. In this regard, low-cost transition metal-based electrocatalysts, especially those derived from the metal-organic framework (MOF) present a new class of high-performance electrocatalysts due to their unique physicochemical properties. In this study, freestanding and 3D mesoporous heterostructures of Cobalt/Cobalt-oxide@N-doped carbon with tunable Cobalt valence states hybridized in N-doped carbon matrix on a metal foam substrate were developed through a facile synthesis route, and evaluated for OER, HER, and overall alkaline water-splitting activities. The electrocatalysts showed excellent bifunctional electrocatalytic activities demanding low overpotentials and excellent stability for 50 h.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:20

Chair: Je Hyun Bae (Chungnam National University)

Investigation of dual-targeting natural product inhibitors on amyloid protein aggregation

Da Gyeong Hyun, Dongjoon Im, Dongvin Kwak, Gyusub Yoon, Yeonjeong Kim, Sehyun Hwang, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Alzheimer’s disease (AD) is a type of neurodegenerative disease that leads to cognitive dysfunction and memory loss. Senile plaques and neurofibrillary tangles (NFTs) are considered pathological hallmarks of AD, which are generally observed at the interior and exterior of the nerve cells of AD patients. These pathogenic amyloid aggregates are generated by misfolding of amyloid-β (1-42) (Aβ42) and tau proteins, respectively. Thus, several types of research were suggested to discover therapeutic approaches for AD by suppressing the formation of pathogenic amyloid aggregates including small molecules, post-translational modification (PTM), monoclonal antibodies, and rationally-designed peptide inhibitors. However, despite to approval of monoclonal antibodies including Aducanumab and Lecanemab by the U.S. Food and Drug Administration (FDA), the efficacy was still controversial. Therefore, alternative therapeutic strategies against AD are required. Natural products are a type of small molecule, containing compounds and metabolites obtained by living organisms. Most of all, genipin and pyrogallol were noticed as potential therapeutic candidates against AD due to their abilities to alleviate oxidative stress and neuroinflammation. Herein, we discovered the potential of genipin and pyrogallol to suppress amyloid protein aggregation through multidisciplinary biophysical analyses. The compelling results suggest the applicability of genipin and pyrogallol as therapeutic agents against AD by revealing the underlying molecular mechanisms suppressing amyloid protein aggregation.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:24

Chair: Je Hyun Bae (Chungnam National University)

Fabrication of Uniform Gold Nanorods (Au NRs) Using Modular Microfluidic Device

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‘Seed-meditated method’ is a widely used method for synthesizing gold nanorods (Au NRs). In the method, Au seed particles having a size of 2-3 nm are synthesized and then grown into Au NRs in a growth solution. However, it is reported that due to the high reactivity of the reducing agent, uniformly reacting within the reactor when using the batch reactor is difficult, and thus the uniformity of the synthesized Au seed is low. To solve this problem, we fabricated Au seeds using a continuous flow microfluidic module chip reactor. It significantly reduces the time required for material and heat transfer and the distance required for diffusion between materials due to the high surface area-to-volume ratio at a microscale. These features enable a uniform and very fast reaction within a reactor. In addition, the 'modular' microfluidic system has the advantage of being able to easily control experimental conditions such as mixing points by assembling various individual chips that each play a different role.Therefore, a continuous flow reactor was constructed using a 'modular microfluidic device', and the size, uniformity, and reproducibility improvement of the synthesized Au seed by adjusting the relative injection flow rate of the reducing agent and buffer solution and surfactant was conducted. Buffer solution was used for control reactivity of the reducing agent. TEM and UV-vis analysis were conducted to confirm the size and uniformity of the synthesized Au seed. And adding a growth step after the Au seed synthesis, process of nanorods growth will be analyzed in a real-time using flow cell type modular chip

Oral Presentation : **ANAL1.O-23**
Oral Presentation of Young Analytical Chemists Ⅰ
Room 301 THU 10:28
Chair: Je Hyun Bae (Chungnam National University)

Fabrication of Cobalt Nanoparticles with Controlled Morphology as Electrocatalyst for Water Splitting

Dong Hwan Nam, Sumin Kim[1], Seunghyun Lee[2,*]

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The formation of transition metal nanoparticles (NPs) has been extensively studied due to their high surface-to-volume ratio compared to bulk catalytic materials. Metal NPs of different size and shapes have different crystallographic facets and have different fraction of surface atoms on their corners and edges, which makes it interesting to study the effect of metal nanoparticle shape on the activity of various reactions. Especially, some of transition metal nanoparticles are useful in several processes due to their magnetic properties. The synthesis of transition metal NPs involves the reduction of metal ions in solution, typically using a reducing agent, a stabilizing agent, and a solvent. The size, shape, and structure of the resulting NPs can be controlled by adjusting the reaction parameters, such as the concentration of the metal precursor, the type and amount of reducing agents and the reaction temperature. In this study, we synthesize various cobalt nanoparticle and size by liquid phase reduction. Scanning electron microscope, transmission electron microscope, and X-ray diffraction are used to characterize the synthesized NPs. Effect of the size and shape of the nanoparticles for OER activities we are investigated using various electrochemical technique.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:32

Chair: Je Hyun Bae (Chungnam National University)

Quantitative Proteomic Analysis of Human Neutroblastoma Cells Exposed to Particulate Matter

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Particulate matter (PM) is known to be an environmental risk factor that gives rise to deleterious effects on human health. Owing to its chemical components (e.g., polycyclic aromatic hydrocarbons, NO2, SO2, and so on), inhalation of PM might cause diverse diseases, such as, cardiovascular, respiratory, eye, and skin diseases. Until now, PM studies have generally been focused on the circulatory and respiratory systems. In this study, an effect of PM on the nervous system was investigated using PM exposed neuroblastoma cell (SH-SY5Y). Proteins obtained from PM exposed SH-SY5Y were compared with those from normal SH-SY5Y to obtain biomarker candidates. A global quantitative proteomic analysis of two SH-SY5Y samples was performed using isobaric tags for relative and absolute quantification (iTRAQ) based 2D nano-liquid chromatography-electrospray ionization-tandem mass spectrometry. We confirmed that proteins related to neural development were reduced and those related to cell death were increased due to PM exposure.

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

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:36

Chair: Je Hyun Bae (Chungnam National University)

Layer by Layer Cell Separate, LLCS : Beads Throw Split (BTS)

Gyusub Yoon, Yeonjeong Kim[1], Dongjoon Im, Sehyun Hwang[2], Dongvin Kwak, Da Gyeong Hyun, Hugh I. Kim[*]

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This study is to establish an ultra-sensitive quantitative analysis method for tissue layers using Layer by Layer Cell Separate and Liquid Chromatography-Mass Spectrometry (LC-MS) to improve permeability evaluation among chemical/biological active ingredients in human medicines.Medicines are administered to the human body through oral administration, intravenous administration, and mucosal administration. Currently, the drug screening method mainly used is to supply a culture media containing a drug to a target cell in two dimensions, and cannot implement a decrease in drug penetration according to the depth of the tissue with a three-dimensional structure, and accordingly, the drug delivery power can be overestimated. We presented a method using 3D Spheroid, Layer by Layer Cell Separate (LLCS), and LC-MS to improve penetration evaluation through measurement of drug by depth of tissue.In this study, Solid Tumors spheroids will be separated by thickness through Beads Throw Split (BTS) method. The key technology is to break down proteins between and into enzymes, and to separate remaining cell-cell conjugates by using bead. As the bead speed changes depending on the flow rate of the solution and the number of collisions can be adjusted, various conditions such as enzyme concentration, decomposition time, bead type, size, and solution flow rate will be changed to find optimal conditions.With the application of LLCS, the proteins that bind cells between the layers of the spheroids will be broken down and separated without damaging the cells. By using LC-MS to quantify the amount of drug in the extracellular matrix and absorbed in the cell, the permeability and absorption of the drug and target cell can be accurately measured.

Oral Presentation : **ANAL1.O-26**

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:40

Chair: Je Hyun Bae (Chungnam National University)

Synthesis and electrochemical studies of $Zn_3(BO_3)_2$ material as an anode material for Li-ion batteries

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Commercial anode material such as graphite and lithium titanate have good cyclability but relatively lower specific capacity. In contrast, Si-anodes have a very high specific capacity but suffer from large volume change during cycling. Thus, development of safe anode materials with high performance in terms of both cyclability and specific capacity, is crucial for the successful application of Li-ion batteries. In this study, conversion-type anode materials, i.e., transition metal borates, as promising candidates for Li-on storage are evaluated. In particular, $Zn_3(BO_3)_2$ has been synthesized by conventional solid-state reaction method and used as anode material for Li-ion batteries. $Zn_3(BO_3)_2$ is a good material as an anode with a theoretical capacity of 512.5mAh/g. The electrochemical tests using the 2032 type coin cell of the material for Li-ion battery were evaluated after the prepared sample was characterized by X-ray diffraction (XRD) and thermal weight analysis (TGA). The good results of cyclic voltammograms, long cycling, and rate performance validate its usefulness as a stable and high capacity anode material.

Oral Presentation : **ANAL1.O-27**

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:44

Chair: Je Hyun Bae (Chungnam National University)

Upconversion Nanoparticles with Controlled Morphology for Plasmonic Enhancement of Optical Property

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Upconversion nanoparticles (UCNs) consist of hexagonal NaYF4 nanocrystals doped with trivalent lanthanum ions, which absorb low-energy radiation to release higher energy radiation. UCNs with hexagonal phase are the useful structure for emitting strong photoluminescence (PL). In this study, rod-shaped UCNs with hexagonal phase were synthesized and phase transition can be controlled by adjusting the ratio of gadolinium. When the ratio of gadolinium is more than 30 percent, pure hexagonal phase is observed because the effect of phase transition is greater than that of particles growing. UCNs with 30 percent gadolinium have the highest PL intensity because they have the highest phase homogeneity and the largest size. Plasmonic metal nanoparticles have collective oscillations of free electrons on their surface called localized surface plasmon resonance (LSPR). Their integration can improve the fluorescence of the phosphor by the incident electromagnetic field enhancement arising from LSPR. However, quenching effect reduces fluorescence by nonradiative energy transfer. In this study, we coated the mesoporous silica shell using the synthesized UCNs. The thickness of the silica shell was grown to reduce the quenching effect. We synthesized mesoporous silica shell to increase the surface area. Also, attaching plasmonic metal nanoparticles on mesoporous silica-coated UCNs to enhance the plasmonic effect is ongoing.

Oral Presentation : **ANAL1.O-28**

Oral Presentation of Young Analytical Chemists Ⅰ

Room 301 THU 10:48

Chair: Je Hyun Bae (Chungnam National University)

Performance evaluation of thickness-tapered channel in flow field-flow fractionation with field programming

Young Beom Kim, Myeong Hee Moon[*]

Department of Chemistry, Yonsei University, Korea

Flow field-flow fractionation (FlFFF) is an analytical method that can rapidly separate nano to micron-sized particles by sizes without using stationary phase. In FlFFF, the crossflow that is applied perpendicular to the direction of sample migration is closely related with the diffusion of particles and therefore affects both resolution and retention time. Field programming can help separation of large particles by decreasing crossflow rate over time. However, field programming requires an additional high-cost flow controller. In our laboratory, we developed a thickness-tapered channel in which the thickness of the channel decreases along the channel axis, and demonstrated that micron-sized particles can be separated in an increased speed together with the increase of recovery and an expansion of dynamic size range of separation.In this study, we evaluated the performance of the thickness-tapered channel with a conventional channel using field programming with polystyrene latex particles. Larger particles could be separated in the tapered channel, where the inlet thickness (350-100 um) was thicker than the uniform channel (250 um), and particles were separated faster than the uniform thickness channel under the isocratic field conditions. In addition, similar results with field programming were obtained and compared with a thickness-tapered channel.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:00

Chair: Yeonho Kim (Konkuk University)

Harnessing the surface structure to enable high-performance olivine cathode mateirals for Lithium-ion batteries

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

The high-performance cathode materials is often the critical limiting factor in improving lithium-ion batteries (LIBs). Among all the reported cathode materials for LIBs, olivine-type cathodes have received particular attention in the past decade due to their successful commercialization in diversified electric vehicle (EVs). Currently, there is a focus on developing a high-voltage olivine battery to increase energy density, due to its many advantages over conventional batteries. While studies mainly focus on the macroscopic and bulk crystal structure of the olivine materials, our work suggests that the electrochemical performances of the interfacial structures of cathode materials should also be regulated, as they are the confined regions where charge transfer takes place. In this study, a hybrid coating layer containing carbon (C) and $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) has been applied to high-voltage $LiFe_{0.4}Mn_{0.6}PO_4$ and $LiFe_{0.4}Mn_{0.3}Co_{0.3}PO_4$ cathodes. Our investigation reveals that the coated layer simultaneously supplies electrons and enhances Li-ion transportation, greatly improving electrochemical performances, including specific capacity, rate capability, and cycling stability.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:04

Chair: Yeonho Kim (Konkuk University)

Plasmon Meets Palladium: A Synergistic Approach to Photocatalysis with Au@Pd Core-Shell Structures

Suhyun Kim, Jeong-Wook Oh[1,*]

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Palladium is well known for its excellent catalytic properties, but its ability to efficiently harvest UV-Vis range lights is limited. In contrast, noble metal nanoparticles such as Au, Ag, and Cu exhibit coherent oscillations of their electrons in response to incoming light, a phenomenon known as Localized Surface Plasmon Resonance (LSPR). This generates energetic electrons or "hot electrons" that can be used in photocatalysis. In this study, we synthesized multiple Au@Pd core-shell structures to combine their unique properties and create a synergistic nanoparticle in a single heterogeneous nanostructure. We also controlled the thickness of the Pd shell to determine the optimal nanostructure that exhibits the best synergistic catalytic effect. To evaluate this effect, we selected the reductive reaction of 4-nitrothiophenol (4-NTP) to 4-aminobenzenetiol (4-ABT) as a model reaction.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:08

Chair: Yeonho Kim (Konkuk University)

A Fully Integrated, Microfabricated Analytical System for On-Chip Detection Based on Indium Tin Oxide Interdigitated Array Electrodes

Hyeri Jeon, Je Hyun Bae[1], Donghoon Han[*]

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[1]*Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, Korea*

A new strategy for the fabrication of a three-electrode system used in microchip systems is described herein. A standard photolithography method was used to fabricate an on-chip, integrated, three-electrode system with a solid-state reference electrode, an indium tin oxide (ITO) interdigitated array (IDA) working electrode, and an electrodeposited Pt counter electrode. Electroplating conditions, such as the potential and time, were investigated with respect to the stability and uniformity of the electrodeposited films. A solid-state reference electrode was fabricated using an electropolymerized poly-1,3-phenylenediamine (poly-m-PD) layer on a nanoporous Pt surface. The electrochemical performance of the three-electrode system was evaluated using cyclic voltammetry. The experimental results demonstrated that the proposed system could work as a solid-state reference electrode that can be integrated into microchips for miniaturized analytical systems.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:12

Chair: Yeonho Kim (Konkuk University)

Selectivity of electrochemical reactions by adsorption in confined nanoporous electrodes

Hyun Ju Yang, Jinju Kim, Je Hyun Bae*

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In the field of electrochemistry, increasing selectivity is a very important research topic when using electrodes as catalysts or sensors. Nanoporous electrodes are representative electrode materials for diverse applications, such as catalysts and sensors. Selectivity arising from nanoporous structures has been applied to systems using non-faradaic reactions such ascapacitive deionization, electrochemical supercapacitors, and conductometry. Cases applied to Faradaic reactions have been studied mainly based on reactivity and molecular size. Here, we suggest surface adsorption of reactant molecules as another important factor for selectivity.We observed that a non-adsorption reaction was selectively enhanced more than that of an adsorption reaction at nanoporous electrode due to nanoconfinement effect. This finding may provide insights on the effective utilization of nanoporous electrodes as catalysts or sensors.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:16

Chair: Yeonho Kim (Konkuk University)

Investigation of lipidomic perturbations in feces and saliva from lung cancer patients

Bo Young Hwang, **Myeong Hee Moon**[*]

Department of Chemistry, Yonsei University, Korea

Lung cancer is a fatal disease with the highest incidence and mortality. Most lung cancer patients are found in situations that radical surgery is difficult, because of the lack of early diagnosis methods and the difficulty in obtaining invasive samples. Therefore, it is necessary to develop new biomarkers from non-invasive and easily available samples.Lipid profiling for diagnostic purposes has become one of the promising area in relation to metabolomic approach. Nevertheless, studies of fecal and salivary lipids as potential biomarker candidates have not been thoroughly investigated. Feces and saliva from patients with lung cancer may have significant alterations in lipid profiles. Therefore, lipidomic analysis of fecal and saliva samples from patients with lung cancer is necessary.In this study, lipid profiles of fecal and saliva samples from lung cancer patients (LC, n = 26) together with controls (C, n = 22) were analyzed by nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Total 206 lipids were identified and 166 lipids were quantified in feces, while total 634 lipids were identified and 304 lipids were quantified in saliva. As a result, in fecal samples, PC, PG, Cer, and CE lipids increased in LC group. On the other hand, PI and DG lipids showed decrease in the LC group. While most lipids in saliva were decreased in the LC group, DG and TG lipids were increased in the LC group. Among the lipids showing significant changes, 6 lipids in feces and 36 lipids in saliva were finally determined as biomarker candidates.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:20

Chair: Yeonho Kim (Konkuk University)

Multipods Silica for SERS-active Substrate Application by Gold Coating

Jaejun Park, Seunghyun Lee[1,*]

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[1]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*

Recently there have been significant research interests in the design of plasmonic metal nanoparticle structures due to their unique optical and electrical properties dominated by the collective oscillations of free electrons in the metal, known as surface plasmons. Plasmonic metal nanostructures with unique geometric nanostructures can amplify surface-enhanced Raman scattering (SERS) signals by generating strong localized surface plasmon resonance and hot spots. We synthesized multipods silica nanoparticles in a one-pot method which has many bumps on the particle surface. The multipods silica nanoparticle's shape had affected by sodium halide ions. We made gold-coated multipods silica nanoparticles and investigated their surface morphology and SERS effect using scanning electron microscopy and Raman spectroscopy. Further, the finite element method (FEM) simulation (COMSOL Multiphysics 5.6, Waveoptics Module) showed a higher signal in the electric field of the gold-coated multipods silica nanoparticle. Our study, thus, demonstrates that the gold-coated multipods silica nanoparticles can be used as potential SERS-active substrates for various diagnostic and sensing applications.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:24

Chair: Yeonho Kim (Konkuk University)

Synergistic strategy of europium-doped magnetoplasmonic nanoparticles for aqueous copper(II) sensing

My-Chi Thi Nguyen, Huu-Quang Nguyen, Jaebeom Lee*

Department of Chemistry, Chungnam National University, Korea

Luminescent lanthanide compounds are of interest in imaging, sensing, and catalysis applications owing to their sharp emission and high resistance to photobleaching. Here, europium ion was doped into hybrid magnetoplasmonic nanoparticles which inherit high photoluminescence efficiency and strong magnetic characteristic. The incorporation of fluorescent lanthanide and Ag@Fe_3O_4 nanoparticles has effectively boosted photoluminescence, attributed to the existence of core-shell structure and plasmon silver core. The as-synthesized NPs exhibit as a sensing probe in environmental technology because photoluminescence is selectively and sensitively quenched when encountering copper (II). This heavy metal ion can be possibly removed by intrinsic magnetic NPs. These results suggest that the complex of Eu-doped magnetoplasmonic NPs can be assigned to be an effective sensing material for aqueous copper(II).

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:28

Chair: Yeonho Kim (Konkuk University)

Toxicological Effects of Microplastic Fibers from Different Disposable Face Masks on Soil Nematodes

Jonghyun Kim, Sunghwan Kim[1], Tae-Young Kim*

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

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

Since the COVID-19 outbreak, disposable masks have been widely implemented as a primary preventive measure to minimize virus transmission. Despite their high usage, there has been limited research on the impact of disposable masks on soil ecosystems. This study aims to investigate the toxicological effects of microplastics from masks on Caenorhabditis. elegans (C. elegans) in the soil media. The toxic effects of microplastics from three types of disposable masks (KF94 mask, medical mask, and particulate respirator) and a polypropylene (PP) reference material on the growth and number of offspring of C. elegans were evaluated. The results showed that the growth of C. elegans was not affected by microplastic exposure. However, significant decrease in the number of C. elegans offspring were observed in KF94 masks and particulate masks when exposed to 0.3% (microplastics/soil, w/w) microplastics. Mass spectrometry-based metabolome analysis revealed distinct metabolic changes between the masks, which were not detectable in phenotype. Alterations in the polyamine biosynthetic pathway, which is involved in reproductive function in C. elegans, were commonly observed in the KF94 mask and particulate respirator exposed groups. On the contrary, the pattern of quantitative changes in metabolites was not identical in the two groups. Analysis of mask extracts using ultra-high resolution MS revealed plastic additives that can be reproductively toxic to C. elegans, such as phthalates, suggesting that various plastic additives may be responsible for reproductive toxicity in C. elegans.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:32

Chair: Yeonho Kim (Konkuk University)

Development of a SERS-based assay platform using CRISPR-Cas12a for sensitive molecular diagnostics of COVID-19

Jisoo Seok, Hajun Dang[1], Jaebum Choo[*]

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Since November 2019, the COVID-19 pandemic is still ongoing globally. The current gold standard for detecting the SARS-CoV-2 target gene is RT-PCR. However, since this technology cannot detect the extracted target gene as it is due to the sensitivity limit of the fluorescence detection method, the amplification process of the target gene using the thermocycling process is needed. To implement amplification-free detection of the SARS-CoV-2 gene, we developed a susceptible SERS detection technology based on CRSIPR-Cas12a. First, SARS-CoV-2 RNA was amplified to double-strand DNA by RT-LAMP and then used as an activator for the trans-cleavage of the Cas12a protein. Subsequently, SARS-CoV-2 was quantified by monitoring the change in Raman intensity when the single-strand DNA immobilized on the Au nanopopcorn substrate was cut by the CRISPR/Cas12a system. This presentation will introduce a CRISPR/Cas12a-based SERS assay platform that can quantify SARS-CoV-2 with high sensitivity.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:36

Chair: Yeonho Kim (Konkuk University)

Electrochemical Reactions Affected by EDL Overlapping in Nanoporous Electrodes

Jinju Kim, Hyun Ju Yang, Je Hyun Bae*

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

When a potential is applied to an electrode in a solution containing an electrolyte, an electric double layer (EDL) is formed as ions having a charge opposite to that of the electrode are gathered around the electrode. The EDL is important because electrochemical reactions take place in the layer. Unlike flat electrodes, the EDL overlaps in nanoporous electrodes. EDL overlapping in nanoporous electrodes has been mainly studied in the charging behavior of ions, and not much in the Faraday reaction. In this study, we explore that electrochemical reaction can be controlled by EDL overlapping in nanoporous electrodes by chronoamperometry. We confirmed that the electrochemical reaction is controlled by electrolyte concentration, measuring time, overpotential, and ionic size because of the EDL overlapping. These findings may provide insight into utilization of nanoporous electrodes as catalysts and sensors.

Oral Presentation : **ANAL2.O-11**
Oral Presentation of Young Analytical Chemists II
Room 301 FRI 09:40
Chair: Yeonho Kim (Konkuk University)

An integrated metabolomics and transcriptomics study in lung from hamster infected by Covid-19 variant viruses

Sunho Lee, Jueun Lee, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Coronavirus (Covid-19) has been continuously prevalent to the present, and as time goes on, the cycle of appearance of variant viruses causing reduction of the effectiveness of the vaccine and having very strong transmission power is getting shorter. However, pulmonary pathologies associated with the infection of Covid-19 variant viruses remain to be understood on systematic molecular levels.In this study, metabolic profiling was performed using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS) to identify metabolic changes in the Delta and the Omicron variants compared to pre-infection. And then, metabolic profiles of lung samples were integrated with whole transcriptomic profiles of lung samples analyzed by RNA-sequencing.As a result of multivariate analysis, principle component analysis (PCA) score plots showed stronger separation between pre-infection and post-infection in the Delta than the omicron in both metabolomics and transcriptomics analysis.In metabolic profiles, tryptophan metabolism and glutathione metabolism were significantly changed in only Delta group, whereas, histidine metabolism was specifically altered in only Omicron group. These metabolic pathways are known to be involved in inflammatory and immune responses. In addition, we observed many immune response gene ontologies related to corona variant viruses.Transcriptome-metabolite network analysis was performed by infection time in each variant group to investigate systematically changed metabolic pathways. Purine metabolism and arginine biosynthesis were significantly changed in both two groups by up-regulating gene and metabolite levels showing greater increases in the Delta group.These data suggest that the delta variant causes significant inflammation in lung tissue and changes the immune system than the omicron variant by regulating transcriptome and metabolome. This study provides useful information for changes of metabolic pathways affected by Delta and Omicron variants, and these pathways could be therapeutic targets for two covid-19 variants.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:44

Chair: Yeonho Kim (Konkuk University)

Real-time multi-dimensional single-particle tracking in solution for single-cell dynamcis by intergrated light-sheet-based super-resolution microscopy

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A multi-functional light-sheet-based super-resolution microscopy (LSRM) was investigated by combining with light-sheet, total internal reflection, differential interference contrast, and super-resolution radial fluctuations modules. The cylindrical lens-based astigmatism method was used to determine the spatial movement (x, y, z), while the rotational angles (azimuth and elevation angles) were triggered by orthogonal polarized illuminations. After the surface functionalization of gold nanorods (AuNRs), the motional and rotational behaviors of native AuNRs and functionalized AuNRs in glycerol were studied. This method showed high localization precision of ~6 nm laterally and ~14 nm axially. The results indicated that surface modification of AuNRs largely affected the translational and rotational diffusions in glycerol, which were attributed to the frictional force and van der Waals forces between the AuNRs and glycerol molecules. This technique can be suitable for studying the movement and rotational behavior of surface-modified nanoparticles in solution and single living cells.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:48

Chair: Yeonho Kim (Konkuk University)

Facile Fabrication of Titanium Dioxide Nanoparticles Encapsulated inside Multi-Walled Carbon Nanotubes and Its Application for Photocatalyst

TaeHyeong Kim, Seunghyun Lee[1,*]

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A facile method fabrication multi-walled carbon nanotubes (MWCNTs) with titanium dioxide nanoparticles has been successfully achieved via solid state reactions. In the previous study, nanocomposites of titanium dioxide particles encapsulated inside multi-walled carbon nanotubes were fabricated and characterized by basic analysis such as transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM). Also, adsorption and decomposition experiments of organic materials were performed to characterize the photocatalytic performance of the fabricated nanocomposites. In this study, additional photocatalytic disinfection experiment was performed. E. coli and MS2 coliphage were used as hazardous materials to be removed, and both showed excellent removal rates. Also, a recycling experiment was performed to confirm repetitive catalyst reusability of the nanocomposites, and an ESR analysis was performed to confirm reactive oxygen species (ROS).

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:52

Chair: Yeonho Kim (Konkuk University)

Abiotic Synthesis of Ribonucleosides under Desorption Electrospray Ionization Configuration

Shihyeon Ryu, Sangwon Cha[*]

Department of Chemistry, Dongguk University, Korea

It has been shown that some chemical reactions can be accelerated over 100 to 106 times in microdroplets compared to bulk solution. Reaction acceleration in microdroplets is thought to be accomplished by various factors such as partial solvation, surface-to-area volume increase, reactant confinement, and so on. Recently, abiotic ribose phosphorylation and synthesis of ribonucleosides has been demonstrated successfully in microdroplets generated by electrospray ionization(ESI). In abiotic synthesis of ribonucleosides, the roles of phosphorylated ribose and magnesium ions were highlighted. In this study, we investigated whether ribonucleosides could be synthesized under heterogeneous catalytic environment with magnesium-rich surface. In order to configure this, desorption electrospray ionization(DESI), liquid extraction-based ambient desorption/ionization technique for mass spectrometry(MS), was employed. First, the homebuilt DESI MS interface was tested against the reaction of Girard's reagent T with ketosteroid that has known to be accelerated under DESI MS configuration. After optimizing DESI parameters with a model reaction, studies on the acceleration of ribonucleoside synthesis were conducted. For example, all reactants except magnesium ion were electro-sprayed onto a magnesium-free or -rich surface to investigate the role of magnesium ion in ribonucleoside synthesis. In contrast to the previous report where all reactants were pre-mixed and sprayed, DESI configuration could confirm stepwise reaction by physically separating one reactant from another. Our results suggest that DESI could enable more detailed and precise observation of the mechanism on acceleration of ribonucleoside synthesis occurring in microdroplets.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 09:56

Chair: Yeonho Kim (Konkuk University)

Metal Interface Damping and Refractive Index Effect Study of Single Palladium Coated Gold Nanorods (AuNRs@Pd) Using Dark-Field Microscopy and Spectroscopy

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

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In this study, we investigated the optical properties of palladium coated gold nanorods (AuNRs@Pd) at the single-particle level using dark-field (DF) method. The AuNRs@Pd were synthesized by in-situ palladium shell epitaxial growth mechanism using CTAB-capped AuNRs, and their structural characterization was carried out by electron microscopes. Afterward, the scattering properties of single AuNRs@Pd were characterized under DF microscopy and spectroscopy. Metal interface damping was observed during the synthesis where the blue-shifting was present during the Pd2+ attachment to AuNR interface. Reduction into Pd induced the red-shifting of the plasmonic scattering spectra. The growth phase of palladium shell alters the peak position due to its aspect ratio changes during synthesis. Localized surface plasmon resonance (LSPR) scattering spectra of the synthesized AuNRs@Pd core-shell showed two broad LSPR peaks at around 624.4(+12.6) nm and 470.8(+1.4) nm that correspond to sub-radiant and super radiant plasmon mode peaks, respectively. Fano resonance was clearly observed as spectral dip at 544.8(+2.9) nm in their single-particle scattering spectra. The plasmon peaks shift were observed in response to refractive index changes, whereas the increment of RI value tends to make both peaks be red-shifted. The position of Fano resonance in response to RI changes is dependent on the thickness of Palladium shell which can bring heterogeneity on LSPR spectrum on each of single nanoparticles. The scattering spectra of thin palladium shell AuNRs@Pd exhibited higher shift sensitivity as a function of refractive index value, where the sensitivity is 2.44 times more on super radiant plasmon peak and 1.55 times more on sub radiant plasmon peak when being compared to the scattering spectra of thick palladium shell bimetallic nanorods.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:00

Chair: Yeonho Kim (Konkuk University)

Uncovering Key Domains for Amyloid-*β* (1-42) Fibrillar Aggregation: Implications for Therapeutic Interventions

Dongjoon Im, Dongvin Kwak, Da Gyeong Hyun, Gyusub Yoon, Yeonjeong Kim, Sehyun Hwang, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Many neurodegenerative diseases have clinical signs that are fibrillar amyloid aggregates. One of the main components of senile plaques in the brains of people with Alzheimer's disease is the amyloid-*β* (1-42) protein, making it a key target for disease therapy. The development of aggregation inhibitors as possible therapeutic medicines depends critically on identifying the key domains of amyloid-*β* (1-42) that enable its oligomerization. In this work, we found three important hydrophobic domains on amyloid-*β* (1-42) and looked into their role in the protein's self-assembly. Based on these discoveries, we created potential amyloid-*β*(1-42) aggregation inhibitor peptides. Utilizing the developed peptides, we investigated the functions of the three hydrophobic domains during amyloid-*β* (1-42) fibrillar aggregation and observed the ensuing impacts on its aggregation behavior and structural conversion. Also, we looked at the interactions between the two C-terminal end residues and the two hydrophobic domains, as well as their functions in amyloid self-assembly, using an amyloid-*β* (1-42) double point mutant (I41N/A42N). Our findings suggest that the central hydrophobic region of amyloid-*β* (1-42) has interchain interactions that are crucial for fibrillar aggregation, and that these interactions affect how accessible the central hydrophobic area is to the start of the oligomerization process. Our research identifies important structural domains that aid in the self-assembly of amyloid-*β*(1-42) and offers mechanistic insights into how it occurs. These findings can also be used to enhance the rational design of potential amyloid-*β*(1-42) aggregation inhibitors.

Oral Presentation : **ANAL2.O-17**
Oral Presentation of Young Analytical Chemists II
Room 301 FRI 10:04
Chair: Yeonho Kim (Konkuk University)

Highly Sensitive 3D SERS-Active Substrate with Abundant Hot Spots for Detection of cTnI Biomarkers

Sunghoon Yoo, Seunghyun Lee[1,*]

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Immunoassays using surface-enhanced Raman scattering (SERS) for biomarker detection have become an active research field due to their high sensitivity and selectivity. In this study, 3D SERS-active substrate with abundant hot spots was developed for the detection of biomarkers. Nickel foam with a three-dimensional(3D) structure provided a large specific surface area. SERS substrate with hot spots was formed by gold deposition after making nanostructures with surface modification through thermal. As a result, we were able to detect MGITC, Raman reporter, at a very low concentration(10e-10 M), indicating the high sensitivity and reproducibility substrate. In addition, we conducted a competition assay using 50 nm-sized gold nanoparticles and 3D SERS-active substrate, and the limit of detection of cTnI was determined to be 1 pg/mL. The 3D SERS-active substrates with abundant hot spots have the potential to be used as a sensitive and selective tool for the detection of various biomarkers in complex biological samples.

Oral Presentation : **ANAL2.O-18**
Oral Presentation of Young Analytical Chemists II
Room 301 FRI 10:08
Chair: Yeonho Kim (Konkuk University)

Highly Sensitive and Label-Free Detection of Influenza H5N1 Viral Proteins Using Affinity Peptide and Porous BSA/MXene Nanocomposite Electrode

Ji Hong Kim, Jong Pil Park[*]

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

Influenza viruses can cause pandemics through animal-to-human and inter-human transmission. Neuraminidase (NA), a glycoprotein on the surface of influenza A and B viruses, is a promising candidate for testing due to its minor immunogenicity. We used phage display to identify an affinity peptide specific to the influenza H5N1 virus NA, which was assessed for its binding affinity via enzyme-linked immunosorbent assay (ELISA). Four synthetic peptides were chemically synthesized and tested to develop an affinity peptide-based electrochemical biosensing system. Among the peptides tested, INA BP2 peptide was selected as a potential candidate and subjected to square wave voltammetry (SWV) for evaluating its detection performance. To enhance the analytical performance, we applied a three-dimensional porous bovine serum albumin (BSA)–MXene (BSA/MXene) matrix. The surface morphology of the BSA/MXene film-deposited electrode was analayzed using X-ray photoelectron spectroscopy (XPS), field-emission scanning electron microscopy (FE-SEM), and electrochemical measurements (CV and EIS). The BSA/MXene nanocomposite-based peptide sensor showed a significant dissociation constant (Kd = 9.34 ± 1.20 nM) and a low limit of detection (LOD, 0.098 nM) using SWV measurement. The sensor exhibited good reproducibility, stability, and recovery, even in the presence of human plasma. Our study demonstrates a new bioanalytical sensing platform for developing highly sensitive virus detection methods.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:12

Chair: Yeonho Kim (Konkuk University)

Determination and Analysis of Functional Ingredients in Various Forms of Camaecyparis obtusa(Pyeonbaek) Products by Gas Chromatography-Mass Spectrometry

Minjoo Jeong, Sangwon Cha*

Department of Chemistry, Dongguk University, Korea

Natural complex substances(NCS) of plant origins have been widely used by themselves or as additives to household chemical products. Essential oils are representative forms of NCS and they are often listed in the international organization for standardization(ISO) along with their constituents and contents. However, some of the essential oils we regularly use are not included in the ISO. In case of evaluating the products containing these non-ISO listed essential oils for registration purposes, we face difficulties because it is hard to clearly define the functional components of the corresponding essential oil. In this study, we tried to construct a strategy for determining functional ingredients of non-ISO listed essential oils by employing both text-mining approach and chemical analysis. For this purpose, we selected an essential oil of Camaecyparis obtusa (pyeonbaek) as a model. First, we investigated functional components of pyeonbaek oil and their contents through literature search. Then, we performed quantitative and qualitative analysis of several pyeonbaek oil products by gas chromatography-mass spectrometry (GC-MS). Through this approach, we could determine about ten functional ingredients of pyeonbaek oil. In addition, we also developed and performed chemical analysis for pyeonbaek oil-containing products such as a tooth paste and an oral spray by using direct injection or headspace GC-MS, and evaluated them in terms of contents of determined functional ingredients.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:16

Chair: Yeonho Kim (Konkuk University)

Investigation of enzymatic oxidation mechanism of model lignins using LC-ESI-MS/MS

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There are growing demands for the valorization of lignin into depolymerized aromatic chemicals. In our previous work, enzymatic oxidation using laccase, a multicopper oxidase, was reported to produce valuable benzaldehyde chemicals from plant lignin, but the mechanism of transformation remains unknown. To understand the mechanism of laccase-mediated oxidation of lignin, the oxidation products of lignin model dimers with three different linkage types (G(8-O-4)G, G(8-5)G, and G(8-8)G) were characterized using liquid chromatography-electrospray ionization-tandem mass spectrometry coupled with a UV detector for selective detection of aromatic chemicals. Under laccase treatment for 24 h, 69%, 61%, and 89% of G(8-O-4)G, G(8-5)G, and G(8-8)G model dimers were transformed into oxidation products, respectively. The abundance of an aldehyde-functionalized oxidation product (m/z 713.2595, 2(G(8-5)G+CH2O)) of G(8-5)G was increased six times compared with the control sample without enzyme treatment, whereas the abundances of aldehyde-functionalized products of G(8-O-4)G and G(8-8)G were unchanged. MS/MS spectrum of the aldehyde-functionalized oxidation product (m/z 713.2595, 2(G(8-5)G+CH2O)) revealed the neutral losses of two aldehyde groups (CH2O and 2CH2O, m/z 30.01 and 60.02). Collectively, these results suggest that the enzymatic transformation of lignin into benzaldehyde chemicals could be associated with the oxidation of (8-5)-type lignin linkage.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:20

Chair: Yeonho Kim (Konkuk University)

Nanoplasmonic assay platforms for reproducible SERS detection of Alzheimer’s disease biomarker

Hajun Dang, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

With the recent developments in high-sensitivity optical detection technologies, many studies have been conducted to accurately detect biomarkers with low concentrations of 1.0 pM or less and apply them to in vitro diagnostics. The tubulin-associated unit (tau-381) protein, a biomarker of Alzheimer's disease, is a representative example, and its cut-off value reported in clinical practice is 5.5 fM. Therefore, a robust sensing technology that detect such low concentrations of biomarkers is needed. In this study, tau-381 was detected with high sensitivity and reproducibility by a plasmonic Au nanopopcorn substrate fabricated via thermal evaporation. Here, aptamer DNAs labeled with Raman reporters on the terminal were used as the receptors. The plasmonic nanopopcorn substrate used in this study is composed of uniform gold nanoparticles (AuNPs) of an average size 64 nm. The reproducibility was significantly improved through more uniform nanogaps than those formed by aggregation of AuNPs in solution. An assay was conducted by first reacting tau-381 with the corresponding aptamers, and the remaining aptamer DNAs were then reacted with capture DNAs immobilized on the surface of the Au substrate. The assay results for tau-381 showed a detection limit value of 2.2 fM, below the cut-off value (5.5 fM).

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:24

Chair: Yeonho Kim (Konkuk University)

Fabrication of Porous Polymer Shell on Carbon Sphere and Application for Catalyst

Chae Yeon Lee, TaeHyeong Kim, Seunghyun Lee[1,*]

Department of Applied Chemistry, Hanyang University, Korea
[1]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*

Photocatalysis is a promising technique with many applications, such as renewable energy production and treatment of environmental pollution. Titanium dioxide is one of the most widely researched photocatalyst, but has low efficiency and narrow light response range. So, combining titanium dioxide with porous carbon materials can enhance photocatalytic activity due to many advantages such as high surface area, large pore volume, accessible interior spaces. As a result, porous shell on carbon sphere can be applied to the photocatalyst with good performance. In this study, we synthesized mesoporous polydopamine coated resorcinol formaldehyde carbon (RFC) nanoparticles. First, a facile method fabrication RFP sphere with from 100nm to 600nm in diameter has been successfully achieved via sol-gel process which can control particle size. Second, we can be obtained porous nanoparticles coated porous polydopamine shell. Third, we fabricated porous polydopamine shell on carbon sphere by converting polymer into carbon through calcination. Consequently, due to porous polydopamine shell, it can be used as a photocatalyst by forming a nanocomposite with titanium dioxide and applied as a catalyst support in various fields by using various metal oxide.

Oral Presentation : **ANAL2.O-23**
Oral Presentation of Young Analytical Chemists II
Room 301 FRI 10:28
Chair: Yeonho Kim (Konkuk University)

Enhanced Detection and Quantitation of Brain-derived Glycolipids using LC/MRM-MS-based Platform

Ji Eun Park, Hyun Joo An[*]

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

Glycolipids enriched on cell membrane microdomains play significant roles in signal transduction, neuronal cell recovery, differentiation, and memory. Experimental evidence for quantitative changes of specific glycolipids in various neurological diseases such as Alzheimer's disease, Parkinson's disease, and epilepsy strongly supports the importance of glycolipids in brain disease pathogenesis and potential treatment. Therefore, analytical methods for absolute quantitation of disease-related target glycolipids are essential for biomarker discovery and disease monitoring. However, glycolipids are amphiphilic substances consisting of a hydrophilic carbohydrate chain and a hydrophobic ceramide moiety, which makes their separation and analysis extremely challenging. Here, we developed a highly sensitive and highly selective absolute quantitation platform based on reversed-phase LC/MRM-MS. First, the organic modifier content of the diluent was increased to improve the solubility of glycolipids, which directly affects data repeatability. We also optimized the ratio of isopropanol in the mobile phase solvent to enhance the instrument repeatability and minimize the increase of column pressure due to isopropanol. As a result, we could determine high sensitivity analysis at the femtomole level and achieve high repeatability within 8% of the CV. The calibration curve was quantitatively linear with a correlation coefficient (R^2) greater than 0.99. This analytical method enables the detection of ng levels of glycolipids per μg of protein in brain tissue. Our glycolipid quantitation platform will be utilized with a high potential for diagnosis and monitoring of glycolipid-related diseases.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:32

Chair: Yeonho Kim (Konkuk University)

Lipidomic analysis of serum exosomes from patients with cholangiocarcinoma by nUHPLC-ESI-MS/MS and FlFFF-ESI-MS/MS

Hyeju Yu, Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Cholangiocarcinoma is divided into intrahepatic cholangiocarcinoma and extrahepatic cholangiocarcinoma according to the site of origin. It is necessary to differentiate and diagnose the type of cholangiocarcinoma because the treatment methods are different. However, early detection of cholangiocarcinoma is difficult, and the mortality rate is high within 5 years after diagnosis. Therefore, it is necessary to specify a biomarker candidate group capable of distinguishing and diagnosing cholangiocarcinoma.Exosomes are one of the extracellular vesicles (EVs) that are externally released from cells. Exosome contains lipids, proteins, and nucleic acids of the parent cell and closely related to intercellular communication. Therefore, exosomal lipids can serve as biomarkers of disease. Ultracentrifuge, size exclusion chromatography, and size-based filtration method are used for exosome isolation, but each method has its own strengths and weaknesses. Asymmetrical flow field-flow fractionation (AF4) can be utilized as an alternative method for separating/isolating exosomes according to their size. Since AF4 separates particles and macromolecules only with the interaction of flow streams without utilizing packing materials as in chromatography, a possible sample interaction with stationary phase can be removed when biological particles are considered for separation. In this study, the minimum volume of serum capable of exosome lipid analysis was optimized due to the limited volume of patients' serum sample. Exosome lipid analysis of patients serum was optimized to 0.5 mL of serum. For the top-down lipid analysis of exosomes depending on sizes, a miniaturized AF4 channel was constructed in laboratory in order to directly hyphenate it with mass spectrometry (MS) via electrospray ionization (ESI). First of all, a flow optimization was accomplished to separate particles in the size range of the exosomes (30-100 nm) within 10 minutes by varying channel thickness and flow rate in the miniaturized AF4 channel. Secondly, the miniatured AF4 channel was hyphenated with ESI-MS/MS, and the best ionization

conditions are being optimized by altering the flow rate of the modifier and sheath gas and realigning the position of the HESI -II probe.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:36

Chair: Yeonho Kim (Konkuk University)

Yolk-shell structured carbon coated Fe3BO5 as an anode material for high C-rate lithium ion battery applications

Rajeev Kumar, Jeongin Kim[1], Youngil Lee[1,*]

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

Yolk-shell structured, carbon-coated vonsenite (Fe3BO5) were synthesized by the solid-state method and utilized as conversion-type anode materials. The core consists of vonsenite nanoparticles, while the shell is composed of a defective (partially graphitized) carbon layer. A higher synthesis temperature leads to the formation of larger amounts of metallic impurities as a result of the carbothermal reduction. The electrochemical characteristics of the sample synthesized at an optimum temperature of 600 °C were better than those of the sample synthesized at higher temperatures and without the carbon coating. This can be attributed to the smaller-sized crystallites having the least amount of metallic impurities and a better-formed solid electrolyte interphase (SEI). This optimized sample demonstrated an outstanding reversible specific discharge capacity of 976 mAh g-1 at a current density of 0.05 A g-1. Long cyclability test at an ultra high C-rate of 5 A g-1 outlined the critical role of an effective SEI and carbon coating. The origin of the capacity values higher that the theoretical value of 726.3 mAh g-1 is also investigated. Remarkably, this sample demonstrated electrochemical activity even upto a C-rate of 20 A g-1, thus validating the usefulness of this material as a safe and stable anode for fast charging-discharging Li-ion battery applications.

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

Oral Presentation of Young Analytical Chemists II

Room 301 FRI 10:46

Chair: Yeonho Kim (Konkuk University)

Influence of oxygen plasma treatment on the electrocatalytic activity of AuNRs immobilized on ITO surfaces

Mukunthan Ramasamy, Ji Won Ha[1,*]

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

Surface plasmon resonance (SPR) is a unique property associated with certain metallic nanomaterials (e.g., Au, Ag, Cu). The localized surface plasmon resonance (LSPR) is a collective oscillation of conduction band free electrons in metallic nanostructures due to interactions with light. The LSPR property of metallic nanoparticles has attracted great attention for many applications that include photocatalysis and electrocatalysis. The LSPR spectrum of plasmonic nanoparticles is influenced by the size, shape, composition, and change in refractive index (RI) of the surrounding medium. Anisotropic gold nanoparticles (AuNRs) have broadly tunable size, shape, and structure-dependent optical properties, and have good photostability and biocompatibility. Oxygen plasma is a partially ionized gas consisting of electrons, ions, and neutral atoms/ molecules. Radiofrequency (RF) plasma, a nonthermal plasma is often used to remove surface capping material and to change the morphology of metallic nanoparticles (NPs). In this study, single gold nanorods (AuNRs) of considerable size were immobilized on the ITO surface and exposed to oxygen plasma. We discuss the spectral, structural changes, and electrocatalytic activity of oxygen plasma exposed AuNRs by dark-field (DF) microscopy and spectroscopy, scanning electron microscopy (SEM), and cyclic voltammetry (CV). We address the plasmonic effect on AuNRs and the potential-dependent catalytic activity of plasma-treated AuNRs at the single-particle level.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 207 THU 10:20

Chair: Kwang Yeon Hwang (Korea University)

Chemical strategy toward targeted protein degradation

Hyun-Suk Lim

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

Targeted protein degradation, such as proteolysis targeting chimeras (PROTACs), has emerged as a powerful therapeutic strategy. PROTACs are chimeric molecules capable of recruiting a target protein to an E3 ligase, thereby leading to its ubiquitination and subsequent proteasomal degradation. While PROTACs hold great promise as a therapeutic modality, current technology has limitations. Only a few E3 ligases (e.g., cereblon) are utilized for PROTAC development. Therefore, it is urgent to develop a technology that can induce targeted protein degradation by utilizing new E3 ligases. Here, I present the development of a new strategy for targeted protein degradation via the N-degron pathway. Specifically, we discovered highly potent small-molecule ligands for a E3 ubiquitin ligase involved in the N-degron pathway and demonstrated that bifunctional molecules based on the ligands effectively degraded target proteins of interest and exhibited related functional activities. In addition, I will introduce a novel DNA-encoded library (DEL) technology that enables to screen hundreds of millions of compounds simultaneously to rapidly discover potent protein ligands. Our DEL selection method, along with the newly developed small-molecule E3 ligase ligands, will serve as a highly useful chemical biology tool for the development of molecules for targeted protein degradation.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 207 THU 09:00

Chair: Tackhoon Kim (KIST)

Translation-dependence of cytoplasmic mRNA localization investigated by single mRNA imaging in *E. coli* cells

Soojin Park, Nam Ki Lee[*]

Department of Chemistry, Seoul National University, Korea

It has been discovered only recently that bacterial cells spatially organize mRNAs to regulate their functions like eukaryotes. However, the generality and the underlying mechanism of specific mRNA localization in bacteria are poorly understood. In this work, we discovered that translation acts as a critical factor in the subcellular organization of cytoplasmic mRNA in *E. coli*. We visualized different cytoplasmic mRNAs with and without translation using single-molecule fluorescence in situ hybridization (smFISH). The observed translation-dependence of cytoplasmic mRNA localization varies among genes and highly correlates with the distance between the originated DNA and nucleoid periphery. Our results suggest that translation spatially organizes the cytoplasmic mRNAs towards the proximal nucleoid periphery using chromosome organization as a milestone.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 207 THU 09:10

Chair: Tackhoon Kim (KIST)

Brightening M1 macrophage in rheumatoid arthritis through Gating-Oriented Live-cell Distinction (GOLD)

Heewon Cho, Sun Hyeok Lee, Young-Tae Chang[1,*]

School of Interdisciplinary Bioscience and Bioengineering, Pohang University of Science and Technology, Korea

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

Macrophages are the most plastic immune cells depending on environmental stimuli. They have two representative polarized subtypes of M1 and M2, presenting totally opposite characters. While M1 macrophages have pro-inflammatory activities to combat with foreign materials such as bacteria, M2 are anti-inflammatory cells to heal the wound. Though both macrophages are essential to maintain the homeostasis, it would be problematic if physiologically balanced ratio between M1 and M2 is destroyed. It has been known that the overactivation of M1 could cause chronic inflammation, especially autoimmune diseases such as rheumatoid arthritis. In light of this, monitoring M1 in real time would be intensively required, but it has been challenging. To deal with the matter, we established Luminescent-Carbohydrate (LC) library, reflecting unique M1 metabolic features unlike M2 macrophages. Through image-based screening, we elicited M1 selective probe, CDr17, and deciphered the selective mechanism through overexpressed Glucose transporter 1 (GLUT1) in M1 over M0 or M2, which dubbed as Gating-Oriented Live-cell Distinction (GOLD). We demonstrated the practicability of CDr17 to monitor M1 macrophages in vivo in a rheumatoid arthritis animal model.

Oral Presentation : **LIFE.O-3**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 207 THU 09:20
Chair: Tackhoon Kim (KIST)

Development of a Fluorescent Probe for M2 Macrophages via Gating-Oriented Live-Cell Distinction

Sun Hyeok Lee, Heewon Cho, Young-Tae Chang[1,*]

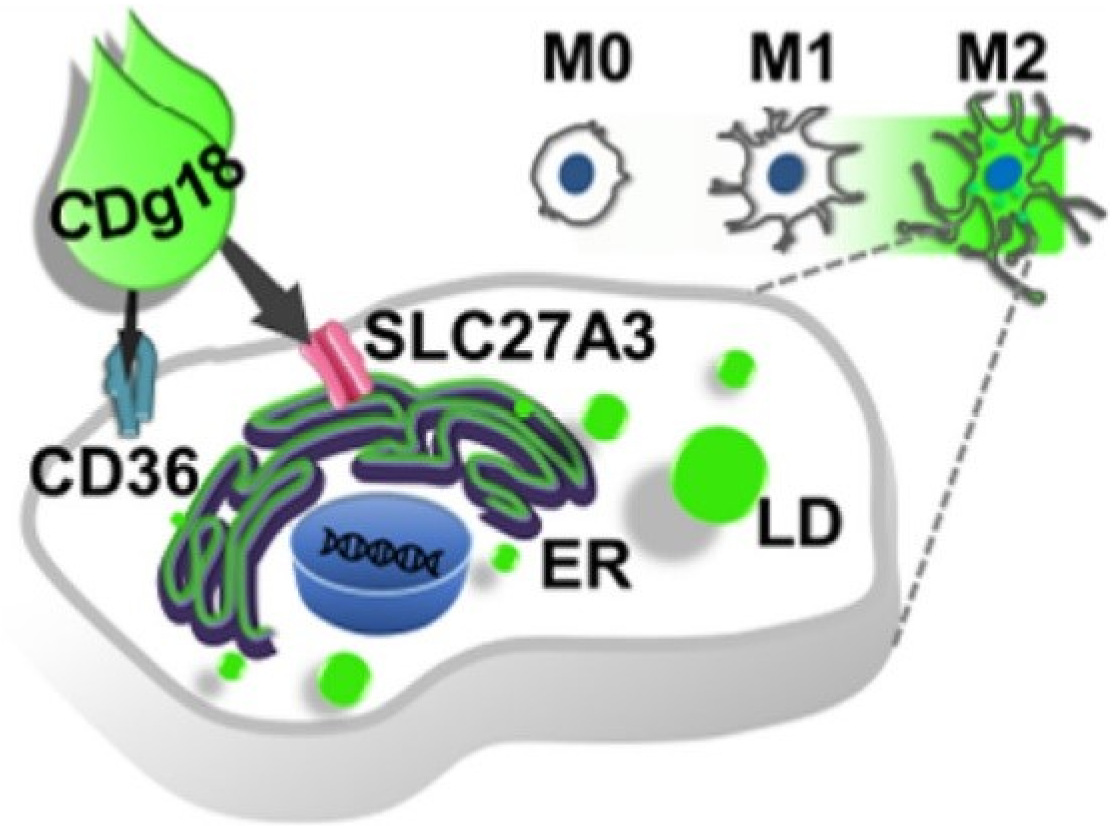
School of Interdisciplinary Bioscience and Bioengineering, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Various types of immune cells exist in the body for the defense system. Especially, macrophage is a type of white blood cell and one of the representative innate immune cells. Macrophages have the plastic phenotype in response to the stimulation from the out of cells, and it is categorized into two different subsets, M1 and M2 type. M1 macrophages are important to pro-inflammatory-related response in the body, and aggressive to offend invaders such as bacteria and tumors. On the other hand, M2 are anti-inflammatory cells, and it is considered as a helper for tumor survival in a tumor microenvironment. It is the reason M2 macrophages are spotlighted in tumor research field. Despite the attractive points as the target, it is lack of monitoring tool for M2 macrophages in the live state.

We developed the first M2 selective probe CDg18, which has fatty acid-mimicked structure, and it was followed with gating-oriented live-cell distinction (GOLD) by fatty acid transporters. The selectivity was originated from the different preference for fatty acid between two types of macrophages. In particular, fatty acid transporter protein 3 (FATP3 a.k.a. SLC27A3) highly expressed in M2 macrophages compared to M0 (pre-differentiated state) and M1 macrophages, and it was verified for the key factor of the selectivity to decrease the fluorescence signal after FATP inhibitor treatment and the target gene removal. To expand the practical application of CDg18, we tried to visualize the phenotype conversion from M2 to M1 macrophages, which is well known drug-induced reprogramming. To achieve the signal change observation by the reprogramming, we exploited the combination of CDr17, previously reported as M1 macrophage-selective probe, and CDg18. After the treatment of a resveratrol analogue HS-1793 as a reprogramming effector, the macrophage reporgramming occurred and the intracellular signal change was observed in the HS-1793 concentration-dependent manner. The fluorophore combination would be suggested as the novel tool for drug screening platform.

Figure. Conceptual scheme for M2-selective probe CDg18.

Ref) J. Am. Chem. Soc. 2023, 145, 2951–2957



Oral Presentation : **LIFE.O-4**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 207 THU 09:30
Chair: Tackhoon Kim (KIST)

Functional nanoparticle probe development incorporated with DNA nanotechnology for biosensor applications

Eunhye Park, Jwa-Min Nam*

Department of Chemistry, Seoul National University, Korea

In order to effectively diagnose cancer and pathogenic diseases, biosensor platforms must satisfy high sensitivity and specificity to respond to target molecules. For a decade, metal nanomaterials have been applied and contributed to biosensor as nanoprobes because the material provides unique optical properties to enhance sensitivity and high binding affinity with biomolecules to increase specificity. Nanoprobe performs target recognition and signal amplification depending on how they are desgined. To extend the functionality of nanoprobes, DNA nanotechnology can be incorporated with nanoprobes for biosensing. Accordingly, the way to exploit nanoprobes is to define a new role of nucleic acids layer on it. Nucleic acids can perform well-defined functions such as signal conversion or target amplification itself as far as the sequence-specific operational roles are concerned. Target sequence transformation is useful when the target strands require high selectivity. For example, single nucleotide polymorphisms (SNPs) are challenging as target nucleic acids because there is only one single base mismatch between the analytes to distinguish specific targets, and the concentration of SNPs in biological samples is low. Consequently, sequences transformation with high-density biomolecules nanoprobes allows similar target sequences to be transmitted to noticeably different sequences via encoding strand amplification. In another case, massively target-strands hybridized nanoprobe can be employed for the target amplification probe itself. To increase the target strand amplification efficiency, the nanoparticle-mediated cycle reaction has been developed under enzyme-free conditions with naked-eye detection.

Oral Presentation : **LIFE.O-5**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 207 THU 09:40
Chair: Tackhoon Kim (KIST)

Spatiotemporal Profiling of Proteins at Membrane Contact Sites by Mutually Orthogonal Protein Labeling and Isolation Systems

Ara Lee, Sanghee Shin[1], Song-Yi Lee[2], Jong-Seo Kim[3,*], Hyun-Woo Rhee[4,*], Kyeng Min Park[5,*], Kimoon Kim[6,*]

Center for Self-assembly and Complexity, Institute for Basic Science, Department of Chemistry, Pohang University of Science and Technology, Korea
[1]*Harvard Medical School, United States*
[2]*Department of Chemistry, Stanford University, United States*
[3]*Center for RNA Research, Institute for Basic Science, School of Biological Sciences, Seoul National University, Korea*
[4]*Department of Chemistry, Seoul National University, Korea*
[5]*Department of Biochemistry, Daegu Catholic University School of Medicine, Korea*
[6]*Department of Chemistry, Pohang University of Science and Technology, Korea*

The identification of dynamic proteins at the contact sites of cellular organelles is essential to comprehensively understand the mechanisms underlying organelle communication and their function. However, current proteomics approaches hinder accurate analysis of such spatiotemporal proteomes. Recently, we developed a new proteomic strategy capable of accurately detecting proteins that are dynamically localized at organelle contact sites. This strategy utilizes two engineered enzymes, TurboID and APEX2, to label proteins close to mitochondria and the endoplasmic reticulum (ER) through biotinylation (Bt) and adamantylation (Ad), respectively. Additionally, two different high-affinity binding pairs, streptavidin (SA)-Bt and cucurbit[7]uril (CB[7])-Ad, were used to selectively enrich Bt- and Ad-labeled proteins orthogonally. The proteomic analysis of Bt- and Ad-labeled proteins resulted in the discovery of new proteins associated with ER-mitochondria contact. Furthermore, it enabled the detection of multiple protein sets undergoing structural and locational changes at mitochondria-associated ER membranes (MAM) during cellular processes such as mitophagy. In this presentation, we will introduce

our recent results that demonstrate the capabilities of a new proteomics tool in identifying spatiotemporal proteins at organelle contact sites and elucidating their dynamic behaviors in vital cellular processes.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 207 THU 10:00

Chair: Tackhoon Kim (KIST)

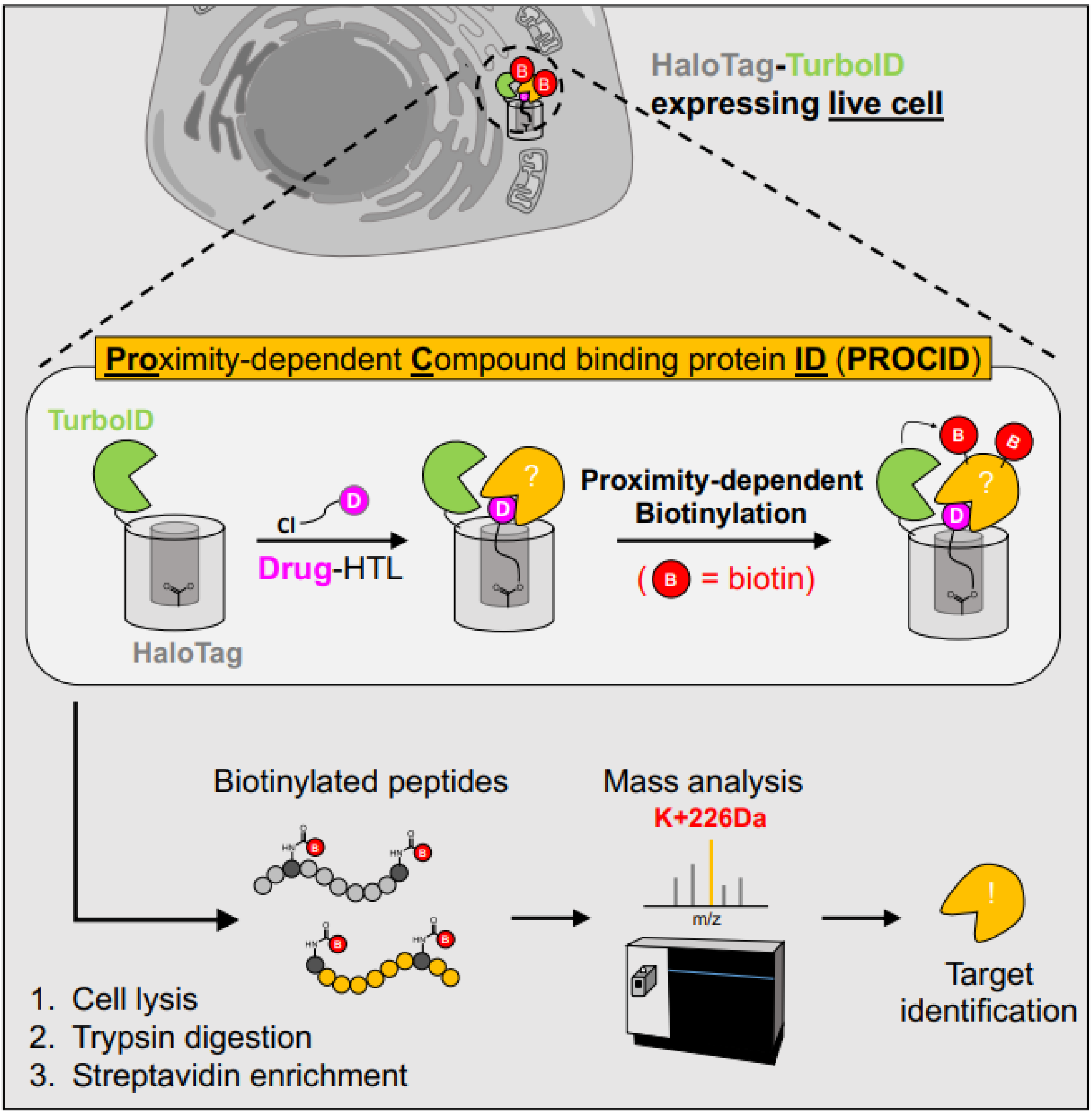
Identification of proteomic landscape of drug-binding proteins in live cells by proximity-dependent target ID (PROCID)

Cheolhun Park, Ho Jeong Kwon[1,*], Hyun-Woo Rhee[*]

Department of Chemistry, Seoul National University, Korea

[1]*Department of Biotechnology, College of Life Science and Biotechnology, , Yonsei University, Korea*

Direct identification of the proteins targeted by small molecules can provide clues for disease diagnosis, prevention, and drug development. Despite concentrated attempts, there are still technical limitations associated with the elucidation of direct interactors. Herein, we report a target-ID system called proximity-based compound-binding protein identification (PROCID), which combines our direct analysis workflow of proximity-labeled proteins (Spot-ID) with the HaloTag system to efficiently identify the dynamic proteomic landscape of drug-binding proteins. We successfully identified well-known dasatinib-binding proteins (ABL1, ABL2) and confirmed the unapproved dasatinib-binding kinases (e.g., BTK and CSK) in a live chronic myeloid leukemia cell line. PROCID also identified the DNA helicase protein SMARCA2 as a dasatinib-binding protein, and the ATPase domain was confirmed to be the binding site of dasatinib using a proximity ligation assay (PLA) and in cellulo biotinylation assay. PROCID thus provides a robust method to identify unknown drug-interacting proteins in live cells that expedites the mode of action of the drug.


HaloTag-TurboID
expressing live cell
Proximity-dependent Compound binding protein ID (PROCID)
TurboID
HaloTag
Cl
D
Drug-HTL
?
Proximity-dependent
Biotinylation
(B = biotin)
B
Biotinylated peptides
Mass analysis
K+226Da
m/z
!
Target
identification
1. Cell lysis
2. Trypsin digestion
3. Streptavidin enrichment

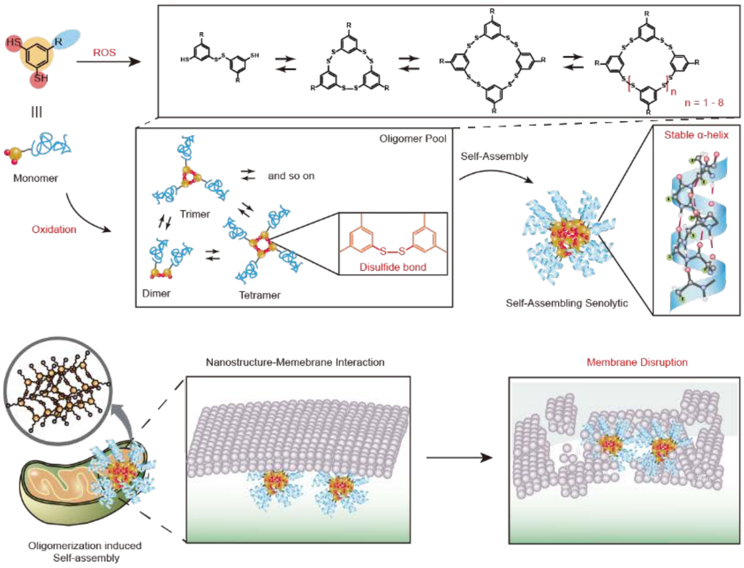
Oral Presentation : **LIFE.O-7**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 207 THU 10:10
Chair: Tackhoon Kim (KIST)

Intramitochondrial polymerization induced self-assembly for regulating cellular fate

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 are synthesized by self-assembly of building blocks such as amino acids, nucleotides, and monossacharides, which leads to construct complex and high ordered structure. The functionality of biomacromolecules is determined by its structure, which sets the foundation for its interaction with other molecules. By mimicking the natural system, we found that formation of disulfide bond give a great platform to form artificial assembled structure for multivalent interaction with bio-macromolecules. Although disulfide bond would be dissociated in intracellular reductive environment, elevated oxidative agents around mitochondria in senescent cells catalyzed formation of disulfide bond between building blocks. As the formation of disulfide bond increase hydrophobicity, the resultant oligomers assembled into spherical structure inside mitochondria. Thereby, assembled structures interact with mitochondrial membrane via multivalent interaction for inducing dysfunction of mitochondria, leading to apoptosis of senescent cells specifically. This polymerization shows great potential for senolytic treatment with selective removal of senescent cells.


HS
R
SH
ROS
n = 1 - 8
Monomer
Oxidation
Oligomer Pool
and so on
Trimer
Dimer
Tetramer
Disulfide bond
Self-Assembly
Self-Assembling Senolytic
Stable α-helix
Nanostructure-Memebrane Interaction
Membrane Disruption
Oligomerization induced
Self-assembly

Oral Presentation : **ORGN.O-1**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 09:00
Chair: Yongseok Kwon (Sungkyunkwan University)

Total Syntheses of Rucaparib via Imino-Stetter Reaction

Jinjae Park, Cheol-Hong Cheon[*]

Department of Chemistry, Korea University, Korea

Rucaparib is a poly(ADP-ribose)polymerase (PARP) inhibitor which was approved by the FDA for the treatment of ovarian and prostate cancers in 2016 and 2020, respectively. Structurally, rucaparib possesses an indole subunit bearing four substituents along its periphery and an additional seven-membered lactam ring between the two substituents at C3 and C4 positions. Since the indole derivative bearing the four substituents at appropriate positions is not readily available, most of the previous syntheses focused on the protocol for the preparation of the tetra-substituted indole derivatives.Consideration of the structural features of rucaparib, we envisioned that the cyanide-catalyzed imino-Stetter reaction recently developed by our group could be an efficient protocol to access tetra-substituted indole scaffold. Based on this idea, we developed two different synthetic routes toward rucaparib. In the first-generation synthesis, meta-fluorobenzoate, currently used in the process chemistry, was converted into 2-aminocinnamic acid derivative via benzylic olefination. The imino-Stetter reaction of aldimine derived from the resulting 2-aminocinnamic acid derivative and aldehyde afforded the desired tetra-substituted indole derivative. The final lactam formation completed the total synthesis of rucaparib in 27% overall yield. We further developed a second-generation synthesis to resolve the issues raised in the first-generation synthesis. The Heck coupling of ortho-iodoaniline derivative with acrylonitrile provided 2-aminocinnamonitrile which was subjected to the imino-Stetter reaction with the aldehyde to provide the desired tetra-substituted indole derivative. Subsequent construction of the lactam scaffold completed the total synthesis of rucaparib in 59% overall yield.

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 09:15

Chair: Yongseok Kwon (Sungkyunkwan University)

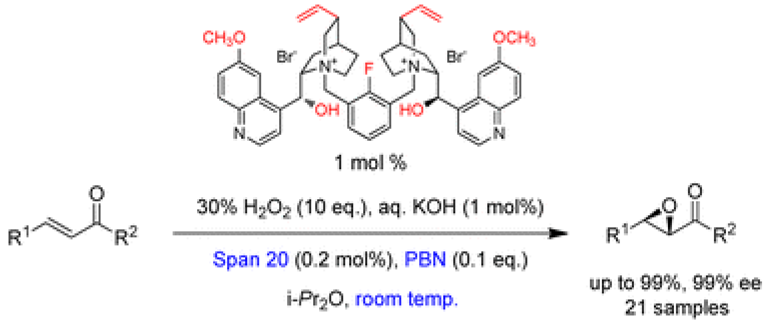
Asymmetric Epoxidation of Enones: Effect of Surfactants and Radical Scavengers on Reaction Rates and Enantioselectivities in Phase-Transfer Catalysis

Geumwoo Lee, Hyeung-geun Park[1,*]

Research Institute of Pharmaceutical Sciences and College of Pharmacy, Seoul National University, Korea

[1]*Research Institute of Pharmaceutical Sciences and College of Pharmacy, College of Pharmacy, Korea*

A highly enantioselective epoxidation of enones has been achieved using asymmetric phase-transfer catalysis (PTC) with *Cinchona* alkaloid-derived *meta*-dimer catalysts. The structure-reactivity relationships among catalysts and oxidants were intensively studied in terms of chemical yields and enantioselectivities, leading to the preparation of optically active epoxides from enones with yields up to 99% and enantiomeric excess (ee) of 99% at room temperature. Additionally, the role of surfactants in the epoxidation process was studied systematically for the first time and was found to play an important role in improving reaction rates and enantioselectivities in asymmetric PTC by forming micellar emulsions that increase the surface area between the organic and aqueous phases when pro-nucleophiles are predominantly in the water phase. Furthermore, the role of radical scavengers and the morphologies of the quaternary ammonium catalysts used in PTC were found to be crucial for ensuring reproducible chemical yields and enantioselectivities in oxidative epoxidations by PTC. The convenient synthesis of the best catalyst and practical PTC conditions make this epoxidation method a suitable choice for industrial applications at room temperature.


CH3O
Br⁻
Br⁻
OCH3
F
N⁺
N⁺
OH
HO
N
N
1 mol %
O
R1
R2
30% H2O2 (10 eq.), aq. KOH (1 mol%)
Span 20 (0.2 mol%), PBN (0.1 eq.)
i-Pr2O, room temp.
up to 99%, 99% ee
21 samples

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 09:30

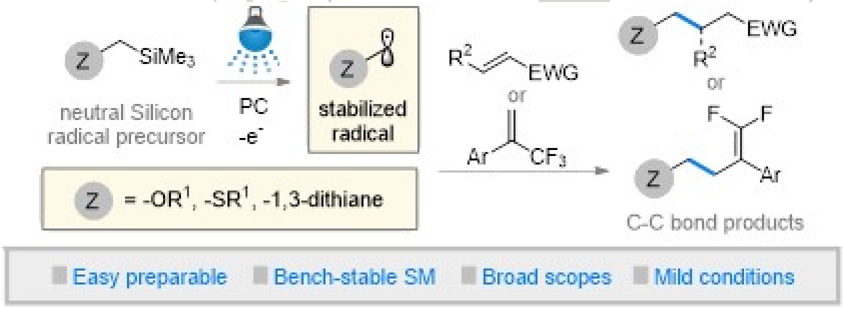
Chair: Yongseok Kwon (Sungkyunkwan University)

Visible-light Induced C-C Bond Forming Reaction using Silicon as a Neutral Radical Precursor

Shafrizal Rasyid Atriardi, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

Visible-light induced C-C bond forming reaction are widely known and represent the pivotal core of organic synthesis. Herein, we report a new strategy for visible-light induced C-C bond forming reaction using α-silyl ethers/thioethers with Michael acceptors and trifluoromethyl alkenes. Various functional groups were tolerated and provided good to excellent yields in mild conditions. A preliminary mechanistic investigation provides evidence for reaction mechanism involving a photoinduced electron transfer.



Oral Presentation : **ORGN.O-4**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 09:45
Chair: Yongseok Kwon (Sungkyunkwan University)

Targeted Protein Degradation of Phosphorylated p38 Mitogen-Activated Protein Kinase (MAPK) as a Novel Approach for the Treatment of Alzheimer's Disease

Seung Hwan Son, Nam-Jung Kim[*]

Department of Pharmacy, Kyung Hee University, Korea

Targeted protein degradation (TPD) has unique advantages over gene knockdown. TPD-based small molecules can induce selective degradation of disease-associated proteins attributed to mutations or aberrant post-translational modifications (PTMs). We used targeted protein degradation as a strategy to induce selective degradation of a disease-associated protein, phosphorylated-p38 (p-p38) mitogen-activated protein kinase (MAPK) in this work. It has been reported that p-p38, which is an active form of p38 MAPK, is significantly upregulated under pathological conditions, then triggering downstream signal transduction and leading to pathological deterioration. Given that the activation of p38 MAPK plays an essential role in the pathophysiology of Alzheimer's disease (AD), selective degradation of p-p38 may provide an attractive therapeutic option for the treatment of AD. Based on the phosphorylation-dependent conformational change in p38 MAPK, we rationally designed and synthesized p-p38 degraders, which selectively bind to an active form of p38 MAPK and induce degradation of p-p38. Among them, PRZ-18002 efficiently degraded p-p38 as well as showed excellent kinase selectivity. In the 5xFAD transgenic mice model of AD, PRZ-18002 reduces p-p38 levels and alleviates microglia activation and amyloid beta (Aβ) deposition, leading to improvement of spatial learning and memory. PRZ-18002 also significantly reduced the p-tau level in the PS19 mice, indicating that PRZ-18002 may ameliorate tauopathy as well as Aβ pathology. Our findings suggest that PRZ-18002 ameliorates AD pathophysiology via selective degradation of p-p38. It provides a novel therapeutic TPD modality that targets a specific PTM to induce selective degradation of the neurodegenerative disease-associated protein.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 10:00

Chair: Yongseok Kwon (Sungkyunkwan University)

A lysosomal NO-selective fluorescent probe enables bioorthogonal exploration of NO involved in autophagy and ferroptosis

Sun Young Park, 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.

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 10:15

Chair: Yongseok Kwon (Sungkyunkwan University)

Synthesis and structure revision of naturally occurring sappanin-type homoisoflavonoids

Sangil Kwon

College of Pharmacy, Gachon University, Korea

Homoisoflavonoids (HIFs) are a subclass of flavonoids with one more alkyl carbon than flavonoids. They are known to have various biological activities, such as anti-angiogenesis and anti-cancer effects. Some HIFs, specifically sappanin type, have been reported to homoisoflavanone containing methyl group in the A-ring or homoisoflavane devoid of a C4 of carbonyl in the C-ring. Dracaeconolide B, a naturally occurring homoisoflavane, was isolated from the red resin of D. cochinchinensis. Efforts have been made to elucidate the exact structure since it was confirmed that dracaeconolide B did not contain a 7-hydroxy-5,8-dimethoxy moiety. The structure of dracaeconolide B was revised by synthesis of three homoisoflavanes containing a 5,6,7-trioxygenated moiety each and analysis by NMR spectroscopy. The revised structure of dracaeconolide B was proposed as 3-(4-hydroxybenzyl)-7-hydroxy5,6-dimethoxychromane. The absolute configuration of the compound was revised to S based on the results obtained by the ECD and optical rotation. We examined the antiangiogenic activity of (S)- and (R)-dracaeconolide B and of synthetic 5,6,7- and 5,7,8-trioxygenated homoisoflavanes. Sappanin-type HIFs possessing methyl substituents on the A-ring have been isolated from L. platyphylla, O. japonicus, P. odoratum, and P. verticillatum. we report the first synthesis of liriopein A and B, as well as other related homoisoflavanones having methyl substituents at the C6 and/or C8 positions. The regioselective A-ring halogenation of 5,7-dimethoxy homoisoflavanone and subsequent methylation via the Suzuki reaction was employed as a key step. The synthetic research of natural products is expected to potentially facilitate the synthesis of related natural products and pharmacological applications.

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 10:30

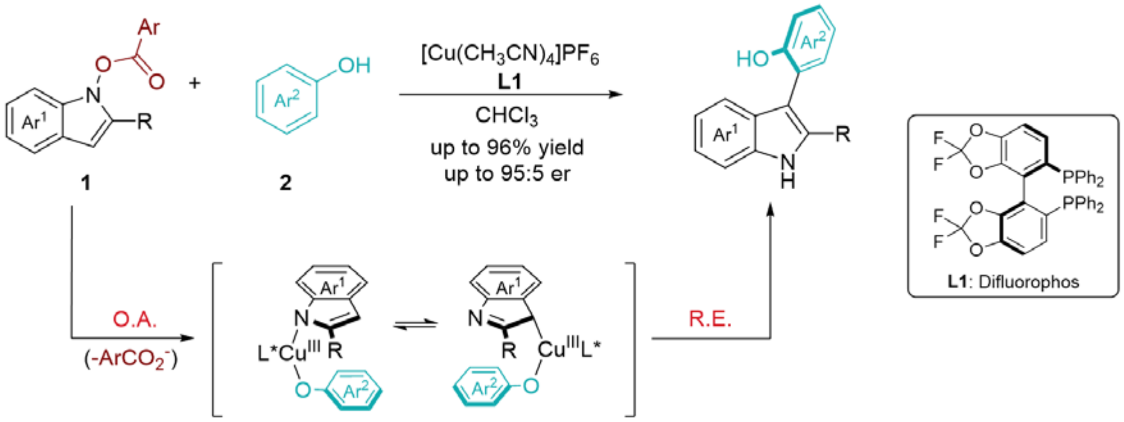
Chair: Yongseok Kwon (Sungkyunkwan University)

Enantioselective Synthesis of Axially Chiral Heterobiaryls from Phenols and Umpoled Indoles

Nguyen Nguyen, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Axially chiral biaryl compounds are commonly found in natural products, bioactive compounds, and chiral ligands.[1] Therefore, heterobiaryl synthesis through C-H/C-H coupling has seen remarkable advances, such as via hypervalent iodine chemistry, electrochemical oxidation, photoredox catalysis and organocatalysis.[2] Despite these advancements, control over chemo- and regioselectivity as well as atroposelectivity remains very challenging.Atroposelective biaryl coupling has been successfully developed through chiral Brønsted acid.[3a-b] However, transition metal-catalyzed process has been rare.[3c] We recently communicated C-H/C-H biaryl coupling protocol employing *N*-carboxyindole (1),[3d] where 27% ee and 54% ee have been accessed through Brønsted acid- or Cu(I)-catalysis, respectively. Herein, we further developed enantioselective C-H/C-H heterobiaryl coupling, by employing Cu(I)/chiral bisphosphine. Through the extensive screening of ligands, we found that (*R*)-Difluorophos ligand (L1) can deliver the desired product in excellent yield (up to 96%) with good enantiocontrol (up to 95:5 er). The current Cu(I)/L1 system turned out to be exceptionally general in terms of phenolic coupling partners.References1 *Nat. Prod. Rep.* 2021, *38*, 1011-1043.2 *Chem. Rev.* 2021, *121*, 4805-4902. 3 (a) *Angew. Chem. Int. Ed.* 2017, *56*, 116-121; (b) *Nat. Chem.* 2018, *10*, 58-64. (c) *Nature Chem.* 2022, doi.org/10.1038/s41557-022-01095-9. (d) *Chem. Sci.* 2022, *13*, 1169-1176.


Ar
O
O
N
Ar^1
R
1
+
OH
Ar^2
2
$[Cu(CH_3CN)_4]PF_6$
L1
$CHCl_3$
up to 96% yield
up to 95:5 er
HO
Ar^2
Ar^1
N
H
R
F
F
O
O
PPh_2
PPh_2
F
F
O
O
L1: Difluorophos
O.A.
($-ArCO_2^-$)
Ar^1
N
L*Cu^{III}
R
O
Ar^2
Ar^1
N
R
Cu^{III}L*
Ar^2
O
R.E.

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 10:45

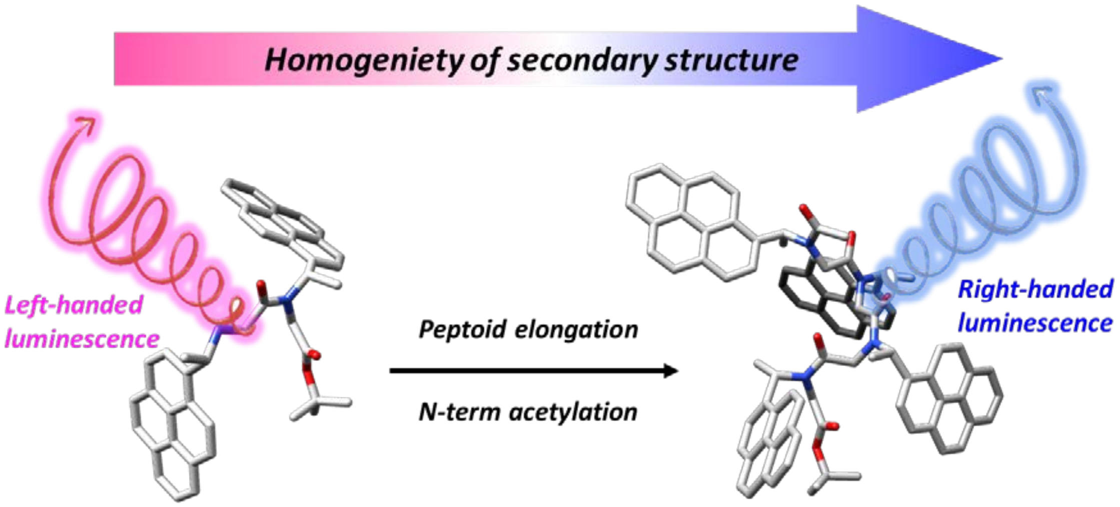
Chair: Yongseok Kwon (Sungkyunkwan University)

Helical display of pyrene on a peptoid: conformational homogeneity induced excimer chirality inversion

Jinyoung Oh, Jiwon Seo*

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

Understanding the relationship between structure and chiroptical properties and controlling the chiral arrangement of chromophores on a helical backbone can be employed to forecast the best materials for use in chiral photonic applications. In this study, we describe the synthesis and structural characterization of an optically active multipyrene system on a peptoid. A systematic structural investigation of pyrene-containing peptoids, as well as their photophysical characteristics, resulting in insights into the relationship between conformational homogeneity and optical activity. The helical propensity of *Ns*1pye oligomers was evaluated through $K_{cis/trans}$ based on NMR spectroscopy, which showed moderate stabilization of *cis*-amide as elongation, and N-acetylation resulted in drastic stabilization. The X-ray crystal structures revealed the progression of the right-handed PPI-like helix, as evidenced by backbone torsion angles similar to previously reported peptoid PPI-like helices. We proposed the interpretation of circular dichroism (CD) spectra when chromophores having complex transitions are CD active. In the case of pyrene, the long- and short-axis-polarized transitions resulted in the opposite tendency of exciton-coupled CD (ECCD) intensity. The excimers generated on peptoids exhibited luminescence dissymmetry related to ground-state homogeneity. Short peptoids tend to emit LCPL and long peptoids with structural homogeneity tend to emit RCPL. Based on the proposed structure-property relationship, our results suggest the chromophore-incorporated peptoid as a promising optically active scaffold for understanding the relationship between structure and optical activity properties, as well as an efficient CPL generator.



H-(*s1pye*)$_2$-COO*t*Bu
X-ray structure

Ac-(*s1pye*)$_4$-COO*t*Bu
X-ray structure

Oral Presentation : **MEDI.O-1**
Oral Presentation of Young Medicinal Chemists
Room 202+203 THU 09:00
Chair: Seong Jun Park (KRICT)

Next-generation Alzheimer's disease therapeutic based on the amyloid hypothesis

Jaehoon Kim, Dokyoung Kim[1,*]

Department of Biomedical Science Graduate School, Kyung Hee University, Korea
[1]*College of Medicine, Kyung Hee University, Korea*

Alzheimer's disease (AD) accounts for more than half of the incidence of dementia and is a disease that causes more and more patients as the aging society progresses. It has been 100 years since AD was first reported in 1906, but even the exact pathogenic substance has not yet been identified. Accordingly, numerous hypotheses about the cause of AD have been reported and studied. Among them, the amyloid-beta hypothesis is one of the hypotheses closest to the correct answer. In this study, we disclosed a new amyloid-beta plaque disaggregation agent and developed a novel therapeutic nanoplatform for AD treatment through brain-targeted moiety surface chemistry of agent-loaded porous silicon nanoparticles (pSiNPs). Based on previous studies, we assumed that the negatively charged sulfonic acid group could bind to amyloid-beta plaques, and based on this, we built a chemical library of 20 compounds. Through in vitro screening, 6-amino-2-naphthalenesulfonic acid (ANA) was derived as a hit compound that can disaggregate amyloid-beta plaques with high efficacy. For the targeted delivery of ANA to the AD brain, we created a nanoplatform using porous silicon nanoparticles (pSiNPs) with ANA loaded into the pore of pSiNPs and biotin-polyethylene glycol (PEG) surface functionalization. As a result, the nanoplatform, named Biotin-CaCl2-ANA-pSiNPs (BCAP), ameliorated memory impairment in an AD mouse model by delivering large amounts of ANA to the AD brain and disaggregating amyloid-beta plaques in the brain. This study presents a novel small molecule for amyloid-beta plaque disaggregation and a promising therapeutic nanoplatform for AD brain-targeted delivery.Ref: Bioactive Materials, 2023, 24, 497-506

Oral Presentation : **MEDI.O-2**
Oral Presentation of Young Medicinal Chemists
Room 202+203 THU 09:12
Chair: Seong Jun Park (KRICT)

Design and Discovery of Macrocyclic compounds as GLS1 Inhibitors for anticancer agents

Krishna Babu Duggirala, Rajath Cyriac[1], Kwangho Lee[2,*]

Medicinal Chemistry and Pharmacology, KRICT, Korea
[1]*Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea*
[2]*Medicinal Chemistry and Pharmacology, Korea Research Institute of Chemical Technology, Korea*

Glutaminase inhibitors are a class of drugs that target the enzyme glutaminase, which plays a key role in the metabolism of glutamine. Glutamine is an essential substrate for many cancer cells, and targeting its metabolism can lead to decreased cell growth and survival. Numerous competitive inhibitors (DON) and allosteric inhibitors (BEPTS, CB-839, etc.) were reported. However to date; CB-839 and IACS-6274 have entered clinical trials. Inhibitors of GLS1 have shown promise in preclinical and clinical studies as potential therapeutics for a variety of cancers, including lung, brain, and ovarian cancer. In this study, we described a series of macrocyclic analogs as selective GLS1 inhibitors. The systematic exploration of the structure-activity relationship by introducing the hydrophilic cyclic linker and different chains based on BPTES led to the discovery of the superior derivative compound 13. Macrocyclic compounds showed excellent potency on GLS1 kinase. Selected molecules resulted in a reduction in intracellular glutamate levels in LR (LDK378-resistant) cells, which is consistent with the cell viability result. Finally, compound 13 selectively reduced the growth of A549 and H460 cells that have cooccurring mutations including KRAS and KEAP1.

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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 09:24

Chair: Seong Jun Park (KRICT)

Exploring Promising A2A Adenosine Receptor Modulators Directly Generated from the Target Protein Structure

Sanghee Yoon, Sun Choi*

College of Pharmacy, Ewha Womans University, Korea

Recent advances in biophysical techniques have increased the availability of three-dimensional protein structures, allowing in silico tools to be used for compound screening and structure-based drug design (SBDD). In addition, artificial intelligence (AI) has emerged as a valuable tool in drug discovery. G protein-coupled receptors (GPCRs), which are located on cell surfaces and transmit signals through cell membranes, have finely regulated dynamics and functions that depend on the type of bound ligands. In this study, we utilized AI model TamGent (Target-aware molecule generator with Transformer) to directly generate compounds for the A2A adenosine receptor (A2AAR) and analyzed their drug-like properties. Docking studies on the A2AAR systems were conducted, examining the residues involved in ligand-binding sites to predict their potential as drug candidates. Furthermore, unsupervised learning methods such as principal component analysis, t-distributed stochastic neighbor embedding analysis, and density-based spatial clustering of applications with noise (DBSCAN) were employed to explore the chemical space of the generated structures. The generated molecules exhibited well-occupied poses that were similar to those of known reference molecules, suggesting the potential for higher binding affinities. Based on these results, TamGent appears to be capable of generating promising drug-like structures.

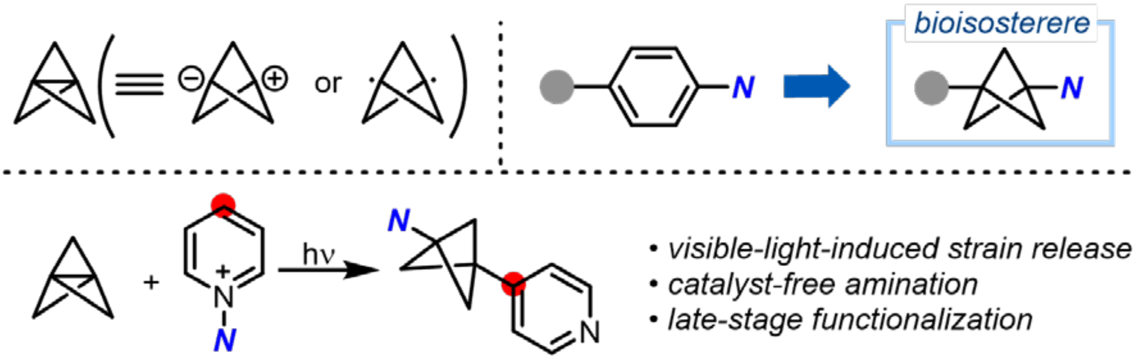
Oral Presentation : **MEDI.O-4**
Oral Presentation of Young Medicinal Chemists
Room 202+203 THU 09:36
Chair: Seong Jun Park (KRICT)

Strain-released amination of [1.1.1]Propellane

Sanghoon Shin, Sungwoo Hong*

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

Replacing an aromatic ring with unconventional bioisosteres can improve the properties of drug candidates while maintaining activity levels. The use of a strained [1.1.1]pentane (BCP) scaffold has gained attention in medicinal chemistry as a nonclassical bioisostere due to its unique structural and conformational rigidity. Especially, the isosteric replacement of aniline is particularly useful to avoid harmful metabolic processes. Bicyclo[1.1.1]pentylamine (BCPA) is a prominent aniline bioisostere that has been extensively studied, offering unexplored drug-like chemical space with varying synthetic utility. A new method of amination of [1.1.1]propellane has been developed, the way of aminopyridiylation was conducted with N-aminopyridinium salts as bifunctional reagents under visible light irradiation. This process allows for directly incorporating amino and pyridyl groups onto BCP frameworks under mild conditions, without needing a photocatalyst. The procedure has a broad substrate scope and offers a convenient tool for creating 1,3-aminopyridylated BCPs. This method expands the scope of BCP-type bioisosteres and has the potential for use in medicinal chemistry.



- *visible-light-induced strain release*
- *catalyst-free amination*
- *late-stage functionalization*

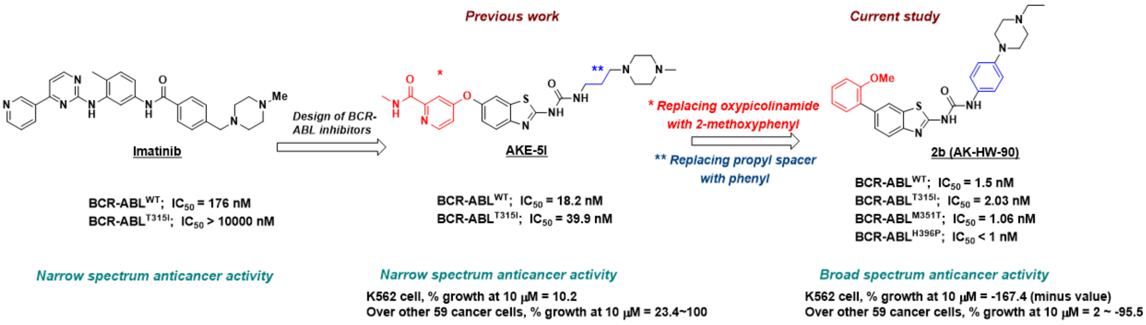
Oral Presentation : **MEDI.O-5**
Oral Presentation of Young Medicinal Chemists
Room 202+203 THU 09:48
Chair: Seong Jun Park (KRICT)

Overriding the imatinib-resistant BCR-ABL mutants with new ureidobenzothiazole chemotypes possessing potent and broad-spectrum anticancer activity

Ashraf El-Damasy

Medicinal Chemistry, Mansoura University, Egypt

The design of kinase inhibitors targeting the oncogenic kinase BCR-ABL constitutes a promising paradigm for the treatment of chronic myeloid leukemia (CML). Nevertheless, the efficacy of imatinib, the first FDA approved targeted therapy for CML, is curbed by emergence of resistance. Herein, we report the identification of the 2-methoxyphenyl ureidobenzothiazole AK-HW-90 (2b), as a potent pan-BCR-ABL inhibitor against imatinib-resistant mutants, particularly T315I. A concise array of six compounds 2a–f were designed based on our previously reported benzothiazoles lead AKE-5l to improve its BCR-ABLT315I inhibitory activity. Replacing the 6-oxypicolinamide of AKE-5l with o-methoxyphenyl, along with changing the propyl spacer with phenyl afforded 2a and AK-HW-90 (2b) with IC50 values of 2.0 and 0.65 nM against BCR-ABLT315I, respectively. AK-HW-90 showed superior anticancer potency to imatinib against multiple cancer cells (NCI) including leukemia K-562. The obtained outcomes offer AK-HW-90 as a promising candidate for the treatment of CML and other types of cancer.



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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 10:00

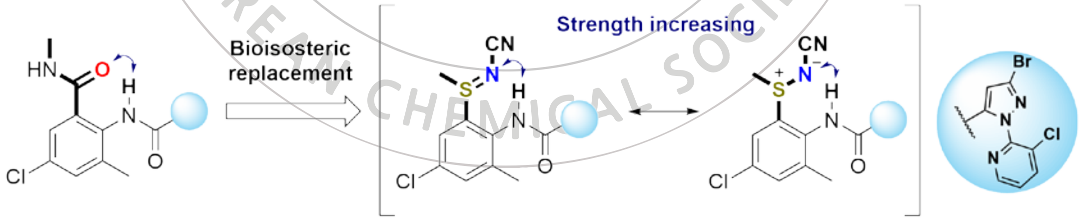
Chair: Ji Young Hyun (KRICT)

N-Cyano Sulfilimine Functional Group as a Nonclassical Amide Bond Bioisostere in the Design of a Anthranilic Diamide Insecticide

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

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

To explore the potential of the *N*-cyano sulfilimine group as an amide bond isostere, a derivative of the blockbuster anthranilic diamide, Chlorantraniliprole, was synthesized and evaluated with regard to its physicochemical properties, permeability, and biological activity. Given the combination of *N*-cyano sulfilimine chlorantraniliprole 1 and its strong hydrogen bond acceptor character, high permeability, and excellent insecticidal activity, the *N*-cyano sulfilimine functional group could be considered as an amide bond isostere.



Chlorantraniliprole
(Rynaxypyr™,Anthranilic diamide,
the blockbuster agrochemicals)

***N*-Cyano sulfilimine Chlorantraniliprole (1)**

: intramolecular hydrogen bonding (IHB)

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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 10:12

Chair: Ji Young Hyun (KRICT)

Plug-and-Playable Mesoporous Silica Nanoparticle For Versatile Targeted Drug Delivery

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

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

For effective drug delivery using nanoparticles, antibody can be beneficially utilized thanks to its high binding affinity to the target site. However, a conventional method to conjugate antibody to nanoparticles involves a multi-step synthetic process, which can damage the antibody’s intrinsic target-recognition nature. Herein, we report a facile approach to construct an antibody-assisted delivery system with high targeting efficiency by achieving direct binding of unmodified pristine antibodies to the nanoparticle surface via simple biomolecular interactions. Mesoporous silica nanoparticles (MSNs) are adopted as a drug-loadable host material, of which external surface is coated with a functional fusion protein consisting of glutathione-S-transferase (GST) and the antibody-binding domain (ABD) called Z domain. It is demonstrated that the Z domain-functionalized MSNs (Z-MSNs) can readily capture antibodies through the Fc regional binding sites and that the antibody-particle binding can be highly stabilized under control of the surface ABD density, against antibody dissociation and exchange with external antibodies. Antibodies can be selectively chosen according to the target and directly applied to Z-MSNs in order to construct a single- or dual-targeting system for enhanced intracellular delivery of pore-loaded drugs to treat cancer. Along with the animal studies showing successful tumoral accumulation and therapeutic activities of antibody-plugged Z-MSNs, the presented results prove a highly facile, efficient, and extensive feature of our delivery platform for a variety of targeted disease treatment.

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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 10:24

Chair: Ji Young Hyun (KRICT)

Therapeutic effect of 5-HT$_7$R ligands on autism spectrum disorders

Jeong Hyun Jeong, Byungsun Jeon, Hyunah Choo[1,*]

Korea Institute of Science and Technology, Korea

[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

Autism spectrum disorder (ASD) is a neurodevelopmental and neuropsychiatric disorder characterized by deficits in social communication and restricted/repetitive behavior. It is very difficult to ascertain the cause of ASD because it has various genetic or environmental causes such as gene polymorphism, viral infection, and dysfunction of neurotransmitters. Serotonin (5-HT) is one of the neurotransmitters, which is implicated in a variety of physiological and pathological processes. Serotonin and its receptors (serotonin receptors, 5-HTRs) are associated with various CNS functions such as behavior, sleep cycles, and cognition. Among 14 5-HTR subtypes, 5-HT$_7$R is most recently dicovered and expressed in the central nervous system (CNS) such as the thalamus, hippocampus, and cerebral cortex, which are closely linked with mental disorder, depression, and ASD. 5HT$_7$R is also involved in the modulation of abnormal neurogenesis, synaptic transmission, and synaptic plasticity in ASD. In this study, we designed and synthesized 5HT$_7$R receptor ligands with biphenyl moiety. We evaluated biological activities of the biphenyl compounds by measuring G protein or β-arrestin activity, followed by determining whether the compounds were agonists or antagonists for 5HT$_7$R. Among the biphenyl compounds, we selected the compound *6h*, which has an antagonistic effect on the β-arrestin signaling pathway as well as G protein signaling pathway. We evaluated the effects of *6h* on repetitive behavior improvement and neurogenesis in ASD. *6h* treatment reduced abnormally-increased self-grooming in shank3 TG mice and increased the number of immature neurons in shank3 TG mice with reduced neurogenesis. Taken together, we suggested that 5HT$_7$R could be a therapeutic target for ASD.

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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 10:36

Chair: Ji Young Hyun (KRICT)

Identification of potent and specific casein kinase 1 epsilon (CK1ε) inhibitors

Injae Shin, Taebo Sim*

Drug Discovery, MagicBullet Therapeutics, Korea

Wnt signaling pathway is overexpressed in colorectal cancers through disruption of adenomatous polyposis coli (APC). Inhibition of casein kinase 1ε (CK1ε) results in supersession of Wnt signaling by interfering with DDX3-CK1ε complex formation and blocking inhibition of Dvl2 phosphorylation. As CK1ε have highly homologous kinase domains with the other five CK1 isoforms (δ, α, γ1, γ2, and γ3) especially Ck1δ, identification of selective CK1ε inhibitor is challenging. In the current effort, we identified potent and selective CK1ε inhibitor SIJ0844 . SIJ0844 displays high potency on CK1ε (IC50 = 14 nM) and selectivity against CK1ε over the other five CK1 isoforms (ratios of the other five CK1 isoforms/CK1ε > 714). Notably, SIJ0844 is superior to PF4800567 in terms of both inhibitory activities and selectivity as well as inhibits only CK1ε among 377 kinases. Moreover, SIJ0844 effectively inhibits autophosphorylation of CK1ε and phosphorylation of its substrate Dvl2. Also, SIJ0844 remarkably induced phosphorylated β-catenin and suppresses c-Myc which are the downstream molecules of Wnt signaling pathway in colorectal cancers cells. Taken together, SIJ0844 as potent and specific CK1ε inhibitor effectively suppresses Wnt signaling on colorectal cancer cells.

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

Oral Presentation of Young Medicinal Chemists

Room 202+203 THU 10:48

Chair: Ji Young Hyun (KRICT)

Discovery of aminopyrimidine derivatives for Toll-like receptor 7/8 agonist as vaccine adjuvant

Sunjong Yu, Chang-Soo Yun[1], Hyejin Kim, Soo Bong Han[2,*]

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

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

[2] *Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

Toll-like receptors (TLRs) are important proteins in pattern recognition receptors (PRRs) that play a key role in the innate immune system response to invading pathogens. TLRs recognize and bind to specific pathogen-associated molecular patterns (PAMPs), triggering a series of signaling pathways that activate immune cells to respond to the pathogen. Human TLRs are classified into 10 types, of which TLR7 and 8 mainly recognize ssRNA fragment derived from virus in the endomal. This ability to stimulate an immune response has led to the exploration of TLRs vaccine adjuvants, which are substances added to vaccines to enhance immune response. We developed new small-molecules as selective TLR7 and 8 agonist. These findings have led to the improved efficacy as a vaccine adjuvant that effectively prevents infection against pathogens.

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

Oral Presentation for Young Material Chemists

Room 405+406 THU 09:00

Chair: Young Jin Sa (Kwangwoon University)

An effective way to enhance the photocatalytic N_2 fixation performance via the optimization of defect structure

Namhee Kwon, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

The defect engineering of nanostructured semiconductor has attracted intense research interest because of its usefulness in exploring efficient N_2 fixation photocatalysts. In this study, the finely controlled defective graphitic-carbon nitride (g-C_3N_4) nanosheets (NSs) were synthesized and employed as cationic building blocks for hybridization with anionic transition metal oxide (TMO) NSs. The resulting 2D superlattice g-C_3N_4-TMO nanohybrids with optimized interfacial interaction and defect structure displayed much higher photocatalytic activity and better selectivity toward visible-light induced N_2 fixation than those of precursor g-C_3N_4 and TMO NSs. The defect-optimized superlattice g-C_3N_4-TMO nanohybrid showed much higher NRR photocatalytic activity than the other superlattices with non-optimal defect contents and disorderly-stacked structure, emphasizing the crucial role of defect control and superlattice formation in optimizing the photocatalytic activity. The excellent photocatalyst performance of defect-optimized 2D superlattice nanohybrid could be ascribed to the strengthening of interfacial electronic interaction, the enhancement of N_2 adsorptivity, and the improvement of charge/mass transport properties.

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

Oral Presentation for Young Material Chemists

Room 405+406 THU 09:15

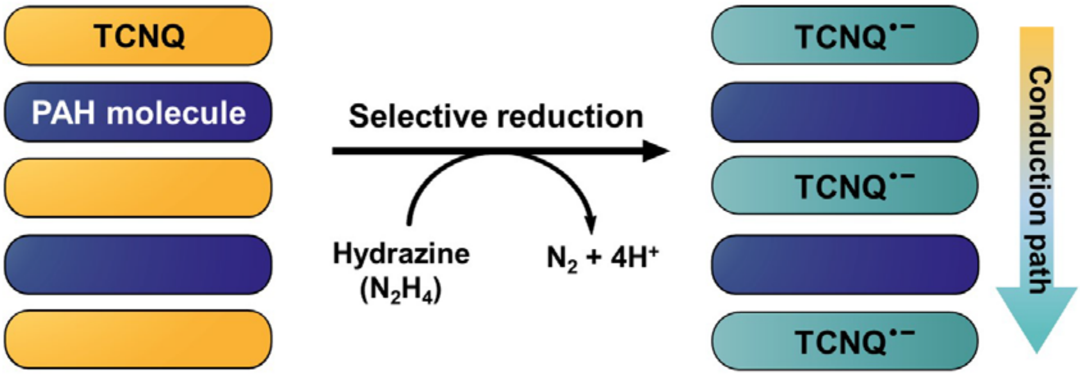
Chair: Young Jin Sa (Kwangwoon University)

Selective Reduction-Induced Molecular Conductors

Hye Soo Kim, Hee Cheul Choi[1,*]

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

Many polyaromatic hydrocarbon molecules (PAHs) are electrically inactive despite their high degree of pi conjugation. We solve this problem through a spontaneous and selective reduction approach to cocrystals including radical-generating molecules as post-treatments, to obtain highly conducting organic crystals. As an example, fluoranthene (FA)-tetracyanoquinodimethane (TCNQ) cocrystals were prepared from mechanochemically prepared FA-TCNQ mixture precursor by the physical vapor transport process. While both FA crystals and as-prepared FA-TCNQ cocrystals show low electrical conductivity, FA-TCNQ cocrystals exposed to hydrazine vapor show dramatically increased conductivity as hydrazine reduces TCNQ to TCNQ radical anions ($\mathrm{TCNQ}^{\bullet -}$) that work as charge carriers in the cocrystals. The systematic studies of electron paramagnetic resonance spectroscopy, Raman spectroscopy, and electrical device measurement support that the generation of radical species from TCNQ by hydrazine reaction is responsible for the high conductivity. Although this strategy requires one extra step toward conducting organic systems than general CT complexes, this strategy is advantageous as it can be applied to any molecules that form cocrystals with TCNQ.



* TCNQ = Radical generator

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

Oral Presentation for Young Material Chemists

Room 405+406 THU 09:30

Chair: Young Jin Sa (Kwangwoon University)

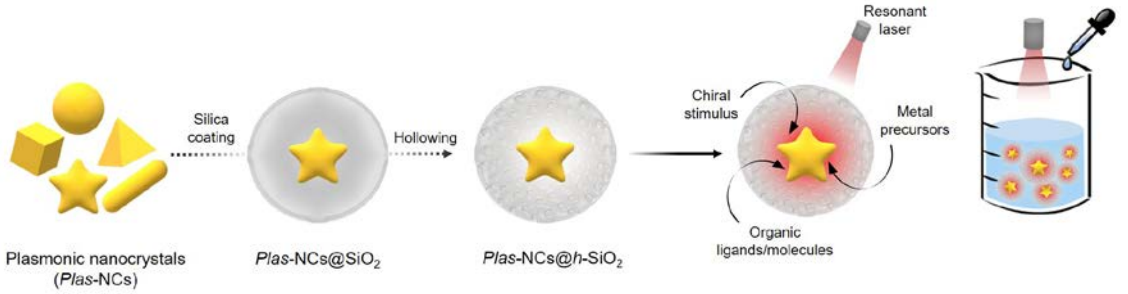
Plasmonic nanocrystals engineering and catalysis using light

Anubhab Acharya, Sampathkumar Jeevanandham, In Su Lee[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

Plasmonic nanocrystals (NCs) are capable to harness light energy and efficiently transform it to carry out catalytic reactions. Therefore, controlling the nanocrystals' shape, size, crystal phase, and elemental compositions can bestow high performance in catalysis. In this context, there is high demand in developing a new solution-phase synthesis technique to precisely modulate the nano-structural features by integrating multiple components into a single nanoscale domain. This strategy creates unique hetero-interfaces such as metal-metal/ligand/support/organic-modifiers to maximize interfacial synergy. To achieve such intricate nanoarchitectures, we introduce a nanoconfinement approach by isolating the individual NCs inside hollow porous silica (called nanoreactors) endowing specific features such as, high stability and surfactant-free NC-surface. This isolated platform has been utilized to elucidate the detailed mechanistic pathway involved in the synthesis process, and the role of excited charge carriers during plasmonic induction by resonant light. Several plasmon induced catalytic transformations are successfully conducted with high efficiency by taking advantage of the unique heterogeneous interfaces originated using this strategy. The prospect of the catalytic reactions in complex intracellular environments has also been studied to demonstrate the wide range of applicability in biomedical science.



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

Oral Presentation for Young Material Chemists

Room 405+406 THU 09:45

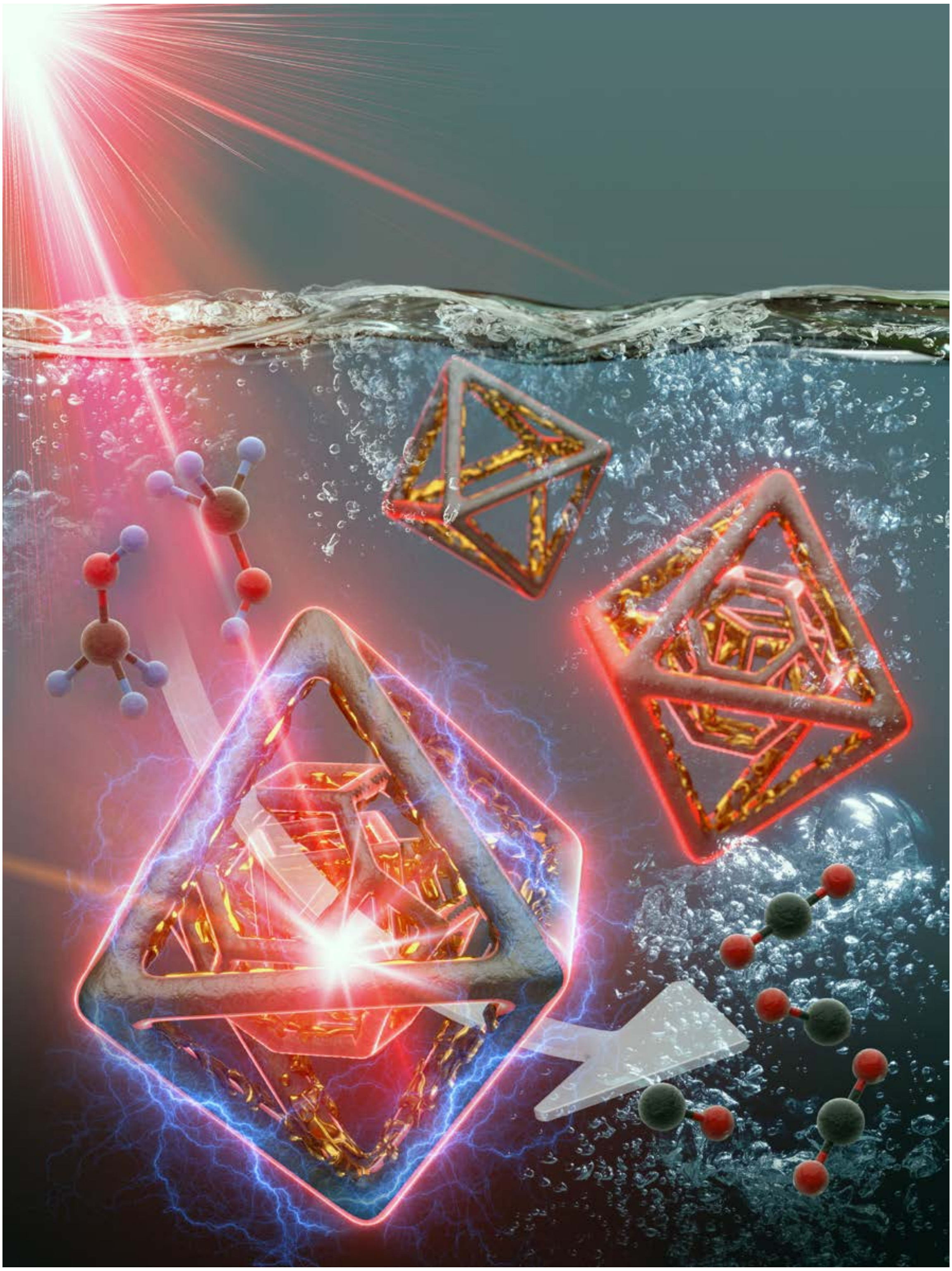
Chair: Young Jin Sa (Kwangwoon University)

Light-Enhanced Electrocatalytic Activity of Multi-Layered PtAu Nanoframes via Plasmonic Hot Spots

Soohyun Lee, Sungho Park[*]

Department of Chemistry, Sungkyunkwan University, Korea

In this research, we demonstrate that the synthetic method of multi-layered PtAu double nanoframes (DNFs) for light-enhanced electrocatalysis which was significantly improved by plasmonic hot spots produced at the nanogaps among multiple nanoframes (NFs) in a single entity. The rational design of complex PtAu DNFs obtained through multiple chemical toolkits was composed of inner truncated octahedral (TOh) NFs and outer octahedral (Oh) NFs with tunable intra-nanogap distances between the NFs. Owing to the plasmonically active Au adatoms on NFs that induce hot carriers under incident light, the electrocatalytic performance toward methanol oxidation reaction (MOR) is significantly enhanced. Remarkably, the hot spots generated from intraparticle plasmon coupling between two adjacent residual Au domains in DNFs greatly boost the electrochemical reaction efficiency. By precisely tuning the gap distances between inner and outer NFs, the correlation of hot spots with electrocatalytic activity was further verified. Additionally, we synthesized hierarchically sophisticated triple NFs (TNFs) which nest one more NF into DNFs, and the resulting TNFs exhibited superior electrocatalytic activity toward the MOR with a 6-fold larger current density under light irradiation compared to the dark conditions due to a high density of hot regions. The exemplified synthetic strategy shows how one can design complex multi-NFs for highly efficient plasmon-enhanced electrocatalysis.



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

Oral Presentation for Young Material Chemists

Room 405+406 THU 10:00

Chair: Young Jin Sa (Kwangwoon University)

Multi-functional Pt_3Rh-Co_3O_4 ternary alloy nanoparticles with superior electrocatalytic activity and long-term stability for alcohol oxidation and water-splitting reactions

Narayanamoorthy Bhuvanendran, **Sae Youn Lee***

Department of Energy and Materials Engineering, Dongguk University, Korea

Developing structure-sensitive electrocatalysts with Pt-rich surfaces consisting of oxophilic metals (Rh) and conductive (carbon) support is vital to boost the electro-oxidation of alcohols. Pt_3Rh-Co_3O_4 ternary alloy nanoparticles of ~2–3 nm were uniformly distributed on carbon (Pt_3Rh-Co_3O_4/C) thru one-pot chemical reduction method. The chemical inertness and oxophilicity of Rh and the abundant oxygen defects of $Co_3O_4$4 improved the kinetics of the methanol oxidation reaction (MOR), ethanol oxidation reaction (EOR), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in Pt_3Rh-Co_3O_4/C by promoting the oxidative removal of surface adsorbed species. Pt_3Rh-Co_3O_4/C exhibits high intrinsic activity for both MOR (6.8 mA/cm^2Pt) and EOR (3.17 mA/cm^2Pt) due to strong electronic, ligand, and bifunctional effects. After 7000 potential cycles (PCs), it retains 81% (MOR) and 84% (EOR) of its initial value, indicating extended stability. In the case of OER and HER, the Pt_3Rh-Co_3O_4 has low overpotential of 290 and 55 mV at 10 mA/cm^2 respectively, which is relatively much lesser than Rh-free catalyst and commercial Pt/C (for HER) and IrO_2 (for OER) catalysts. The durability of the catalysts shows slight shift in the overpotential after 5000 PCs for both OER (+21 mV) and HER (-5 mV) signifies the extended performance in acidic medium. Compared to other Pt-based benchmark catalysts, Pt_3Rh-Co_3O_4/C demonstrates higher CO tolerance, synergistic effect, and good electron conductivity results in extended activity, and stability, corroborate as a potential and competing electrocatalyst for alcohol electro-oxidation and water-splitting reactions.

Oral Presentation : **MAT.O-6**
Oral Presentation for Young Material Chemists
Room 405+406 THU 10:15
Chair: Young Jin Sa (Kwangwoon University)

Incorporating Graphene-Quantum-Dots into Lithium-Sulfur Batteries for Enhanced Electrochemical Performance with Optimized Sulfur Nucleation

Hyeonwoo Cho, Gaeun Bae, Sunhwa Hong, Yung-Eun Sung[1,*], Byung Hee Hong[*]

Division of Chemistry, Seoul National University, Korea
[1]*Division of Chemical & Biological Engineering, Seoul National University, Korea*

Graphene Quantum Dots (GQDs) are 0D materials fragmented into a few nanometer sized particles from larger graphitic materials. GQDs contain a mixture of sp2 and sp3 carbon bonds with various chemical functional groups, exhibiting unique properties such as characteristic fluorescence, quantum confinement effect, amphiphilicity, biocompatibility, etc., which have been utilized to LEDs, photocatalysts, bioimaging and sensing agents, therapeutic agents, and energy applications. Recently, GQDs have been widely used in batteries for their large surface areas and more active sites, resulting in faster charge transfer and ion diffusion. GQDs were also used to address the shuttle effect, a common problem in Li-S batteries, due to their abundant sulfiphilic oxygen functional groups. On the other hand, the failure of Li-S batteries often depends on the sulfur deposition morphology in the cathode, so organic solvents have been introduced to solve this issue, which still limits the performance of the Li-S batteries. In this study, GQDs with abundant oxygen functional groups were introduced into the cathode of a Li-S battery to solve the above mentioned shuttle effect and the sulfur morphology problem, simultaneously. As a result, we confirmed that the overpotential and resistance of the Li-S battery are reduced, and the faster reaction kinetics are observed, indicating that GQDs suppress the shuttle effect and promote the faster charge or mass transfer. Furthermore, we observed minimized capacity fade even after 200 cycles of charge and discharge. In addition, the particle-like morphology of lithium sulfide deposition was obtained, which is advantageous to prevent the formation of sulfur films that degrade the performance of Li-S batteries.

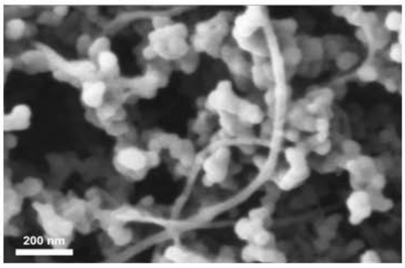


Figure 1: SEM image of the GQD-incorporated cathode of Li-S battery after full discharge.

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

Oral Presentation for Young Material Chemists

Room 405+406 THU 10:30

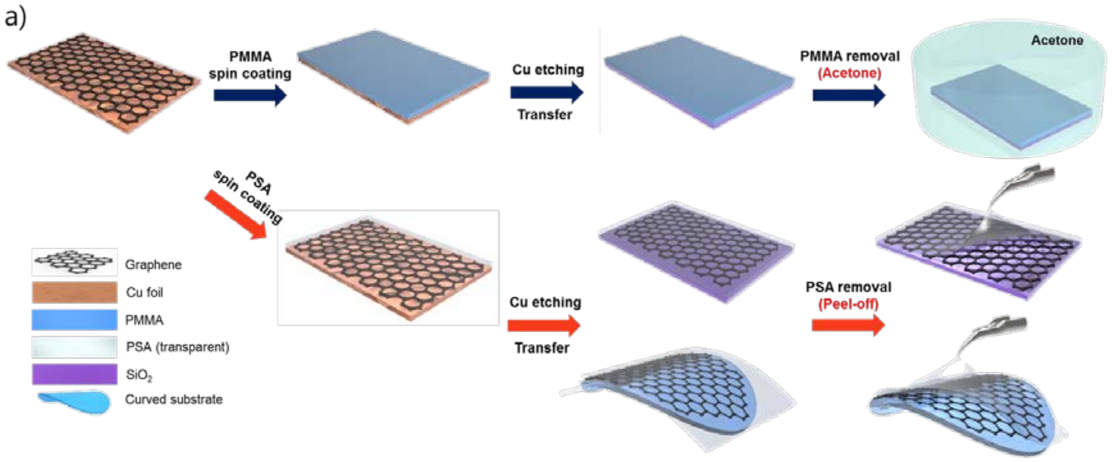
Chair: Young Jin Sa (Kwangwoon University)

A Spin-Coatable Dry Transfer Method of 2D Materials

Yejun Lee, Byung Hee Hong*, Chanjin Kim, HaEun Lee

Division of Chemistry, Seoul National University, Korea

In recent years, researchers have tried to develop various methods to synthesize high-quality large-scale graphene and 2D materials using chemical vapor deposition (CVD) processes. However, transferring and patterning steps during the fabrication of the 2D materials often degrade the electrical performances, because, for example, a conventional transfer method using poly (methyl methacrylate) (PMMA) leaves PMMA residue on the surface of the 2D materials, leading to undesirable doping effect. Moreover, acetone used to remove PMMA damages organic layers. Thermal release tapes (TRT) also cause considerable contamination. Thus, it is needed to develop a new transfer technology to solve the above-mentioned problems.Here, we report a novel transfer method based on the use of pressure sensitive adhesive (PSA) that can be simply spin-coated on the sample, and completely removed by peeling-off after the transfer, which is expected to allow the use of soluble layers for various 2D device fabrication processes. We confirmed that the sheet resistance of graphene has not been altered after transfer thanks to the good adhesion between graphene and PSA layers. In addition, the transparent graphene FETs transferred by PSA shows high charge carrier mobility compared to the FETs transferred by PMMA or thermal release tapes (TRT), implying that the graphene surface is ultra-clean without residues after the removal of PSA. TMDCs including WS_2 and MoS_2 were successfully transferred on a lens for smart glasses applications by PSA with minimized contamination. In addition, using PSA enables simpler patterning process eliminating the need for using photo or e-beam lithography. Thus, we believe that the current method is applicable to various flexible and wearable applications that have been limited by wet transfer conditions for more practical and larger scale device fabrications of 2D materials.


a)
PMMA spin coating
Cu etching
Transfer
PMMA removal
(Acetone)
Acetone
PSA spin coating
Graphene
Cu foil
PMMA
PSA (transparent)
SiO_2
Curved substrate
Cu etching
Transfer
PSA removal
(Peel-off)

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

Oral Presentation for Young Material Chemists

Room 405+406 THU 10:45

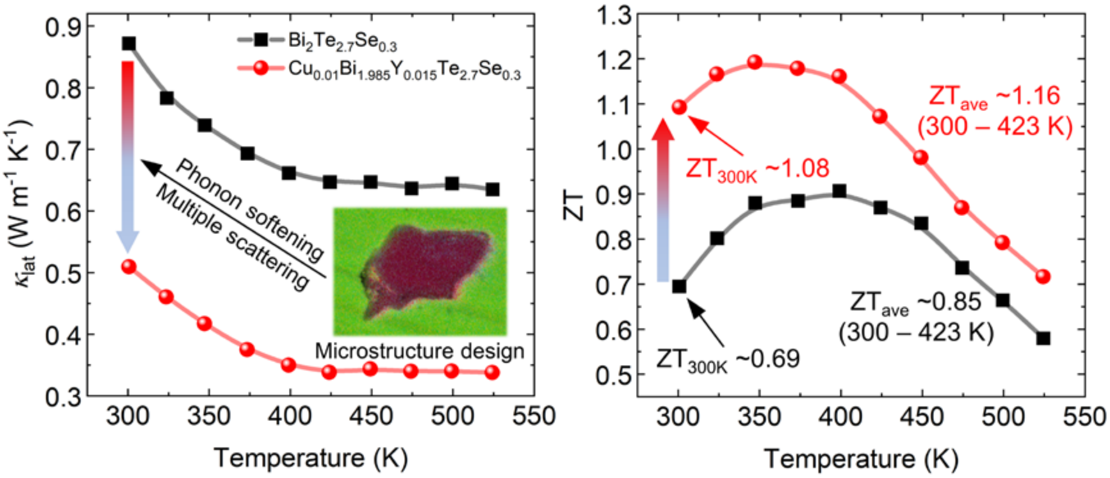
Chair: Young Jin Sa (Kwangwoon University)

High thermoelectric performance in n–type Bi2Te3-based system via unique microstructure design

Hyungseok Lee

Institute of Chemical Processes, Seoul National University, Korea

Bi_2Te_3-based materials have been known for most efficient thermoelectric (TE) material near ambient temperature. However, due to the difficulty in efficient doping and alloying to their structure of Bi_2Te_3, n-type Bi_2Te_3 TE systems have been significantly understudied. Here, we present new n-type $Bi_{2-x}Y_xTe_{2.7}Se_{0.3}$ (x = 0 – 0.020) TE systems and further optimized $Cu_{0.01}Bi_{1.985}Y_{0.015}Te_{2.7}Se_{0.3}$ via unusual yttrium selenide-based microstructures. With altering the incorporated Y content in the system, the composition of the surrounding matrix, microstructures, and their interfaces are simultaneously modulated. The microstructure architecture and compositional tunability via the dual incorporation of Y and Cu atoms can be demonstrated and modulated from the perspective of hard-soft acid-base theory and crystal chemistry of the constituent elements. It effectively supresses the lattice thermal conductivity of the optimized $Cu_{0.01}Bi_{1.985}Y_{0.015}Te_{2.7}Se_{0.3}$ to ~0.51 W m^{-1} K^{-1} system at 300 K. Also, it slightly increases density of states effective mass, inducing enhanced Seebeck coefficients and improved power factor near room temperature, giving ~39.1 μW cm^{-1} K^{-2} at 300 K. Consequently, the $Cu_{0.01}Bi_{1.985}Y_{0.015}Te_{2.7}Se_{0.3}$ system results in a high TE figure of merit, ZT, of ~1.20 at 347 K and an average ZT of ~1.16 from 300 to 423 K.


κ_{lat} (W m^{-1} K^{-1})
0.9
0.8
0.7
0.6
0.5
0.4
0.3
$Bi_2Te_{2.7}Se_{0.3}$
$Cu_{0.01}Bi_{1.985}Y_{0.015}Te_{2.7}Se_{0.3}$
Phonon softening
Multiple scattering
Microstructure design
300
350
400
450
500
550
Temperature (K)
ZT
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
ZT_{ave} ~1.16
(300 – 423 K)
ZT_{300K} ~1.08
ZT_{ave} ~0.85
(300 – 423 K)
ZT_{300K} ~0.69
300
350
400
450
500
550
Temperature (K)

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 09:00

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Design of Naphthalene Diimide for Highly Soluble and Stable Negolyte in Neutral Aqueous Organic Redox Flow Batteries

Vikram Singh, Hye Ryung Byon[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, India

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

Aqueous organic redox flow batteries (RFBs) constitute an emerging energy storage system. Vanadium-based RFBs suffer from rising cost, low abundancy of Vanadium and precipitation of V^{5+} at 40 ^{o}C. Alternatively, Organic redox molecules offer thermal stability, tunable solubility, and redox potentials. Recently, we demonstrated that N, N'-bis(glycinyl)naphthalene diimide (NDI) can show stable two 2e-transfer in aqueous RFBs (J. Mater. Chem. A 2020, 8, 11218, Batter & Supercap., 2022, 5, e202200281). Nonetheless, solubility of NDIs was low (0.7 M) in neutral conditions. Here, we show highly improved solubility of NDI to 1.5 M in water by incorporating tetraammonium groups (ANDI). Around 1 M of ANDI was soluble and stable during the two electron-transfer processes in the absence of precipitation. Electrospray ionization-mass spectrometry, Nuclear magnetic resonance, Electron Paramagnetic Resonance and Molecular dynamics simulations revealed the crucial role of inter- and intramolecular interactions and tetrammonium groups for the stable redox chemistry of ANDI. ANDI molecules formed radical ion–dimers/tetramers during the first reduction process. The structure disassembled to monomeric form during the second reduction process. The aqueous RFBs comprised of 1 M ANDI as the negative electrolyte (negolyte), ammonium iodide as the positive electrolyte (posolyte), and KCl as the supporting electrolyte. The cell showed an average voltage of 1.08 V and stable cyclability 500 times over 45 days. A capacity-fading rate was 0.004% per cycle including negligible crossover through a Nafion 212 membrane. The excellent capacity retention suggested that tetrammonium groups preserved the stability of NDI through multiple electron transfers and long-term cyclability.

Oral Presentation : **ELEC.O-2**
Oral Presentation for Young Electrochemists
Room 205+206 THU 09:15
Chair: Seung-Ryong Kwon (Gyeongsang National University)

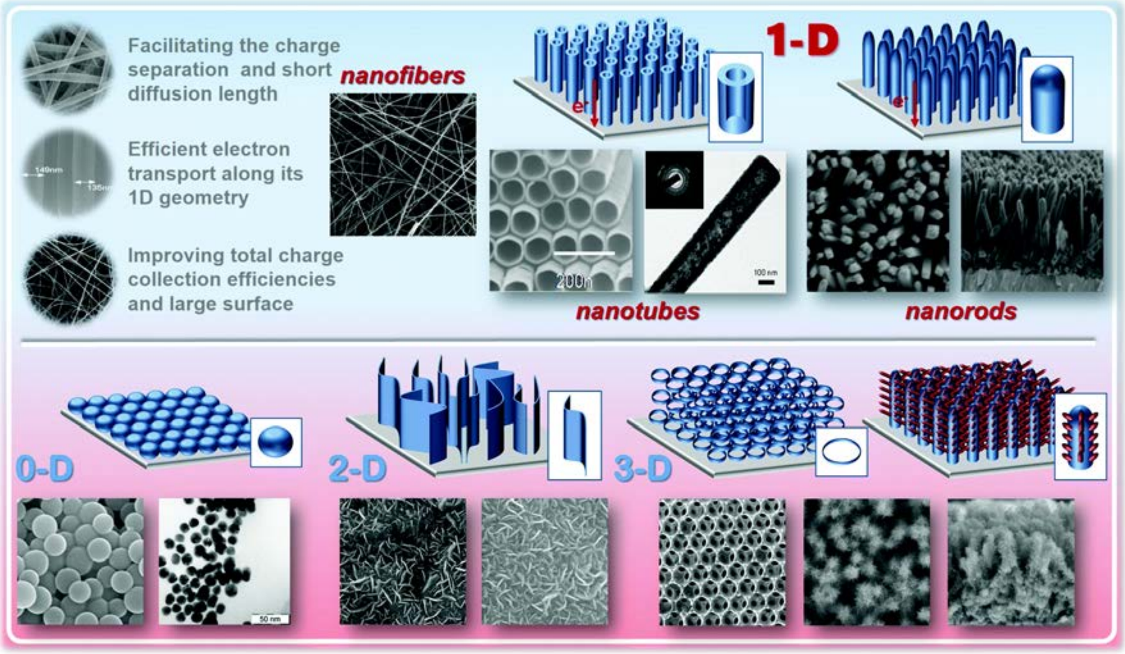
Recent progress on transition metal-based nanostructures for photoelectrochemical water splitting

Goddati Mahendra, Jaebeom Lee[1,*]

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

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

This article gives an exhaustive assessment of current research efforts focusing on zero to three dimensions of transition metal-based nanomaterials (TMNs) for photoelectrochemical water splitting. OD nanomaterials' TMNs consist of nanoparticles, quantum dots, spheres, and hollow spheres. 1D nanomaterials consisting of wires, rods, bands, and tubes All supra-dimensional nanostructures with lateral dimensions between 1 and 100 nm constitute 3D nanomaterials. We focus primarily on 0D–3D nanostructures created in reasonably large numbers by physical and chemical means. This article begins with a review of synthetic methodologies that have been used to accomplish development from 0D to 3D. We then elaborate on these strategies as follows: New ideas that have not been completely proven but have the potential to generate 1D nanostructures in the future Following is a description of methods for producing several kinds of significant heterostructure nanowires. At the conclusion of this article, we will highlight a variety of typical synthesis approaches (e.g., sol-gel methods, hydrothermal methods, template-assisted techniques, self-ordering anodization, and other methods) and typical modification approaches (doping, heterojunction engineering, co-catalyst decoration, and other strategies) associated with various 0D to 3D nanostructures. In addition, we describe briefly a variety of techniques that may be beneficial for combining 1D nanostructures into functional devices based on crossbar connections and sophisticated designs such as 0D and 3D periodic lattices. We end our overview with some personal thoughts on the possible future research avenues for this new class of nanostructured materials.


Facilitating the charge separation and short diffusion length
Efficient electron transport along its 1D geometry
Improving total charge collection efficiencies and large surface
nanofibers
1-D
nanotubes
nanorods
0-D
2-D
3-D

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 09:30

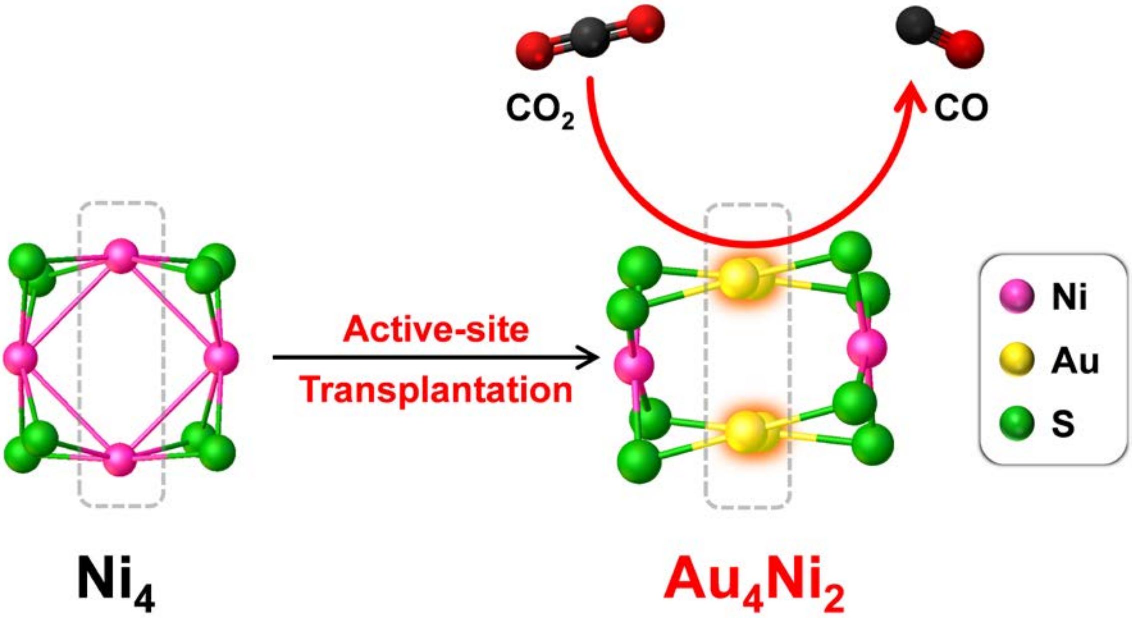
Chair: Seung-Ryong Kwon (Gyeongsang National University)

Transplanting Gold Active Sites into Non-Precious-Metal Nanoclusters for Efficient CO2-to-CO Electroreduction

Yongsung Jo, Dongil Lee[*]

Department of Chemistry, Yonsei University, Korea

Electrocatalytic CO2 reduction reaction (CO2RR) is greatly facilitated by Au surfaces. However, large fractions of underlying Au atoms are generally unused during the catalytic reaction, which limits mass activity. Herein, we report a strategy for preparing efficient electrocatalysts with high mass activities by the atomic-level transplantation of Au active sites into a Ni4 nanocluster (NC). While the Ni4 NC exclusively produces H2, the Au-transplanted NC selectively produces CO over H2. The origin of the contrasting selectivity observed for this NC is investigated by combining operando and theoretical studies, which reveal that while the Ni sites are almost completely blocked by the CO intermediate in both NCs, the Au sites act as active sites for CO2-to-CO electroreduction. The Au-transplanted NC exhibits a remarkable turnover frequency and mass activity for CO production (206 molCO/molNC/s and 25,228 A/gAu, respectively, at an overpotential of 0.32 V) and high durability toward the CO2RR over 25 h.


CO_2
CO
Active-site
Transplantation
Ni
Au
S
Ni_4
Au_4Ni_2

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 09:45

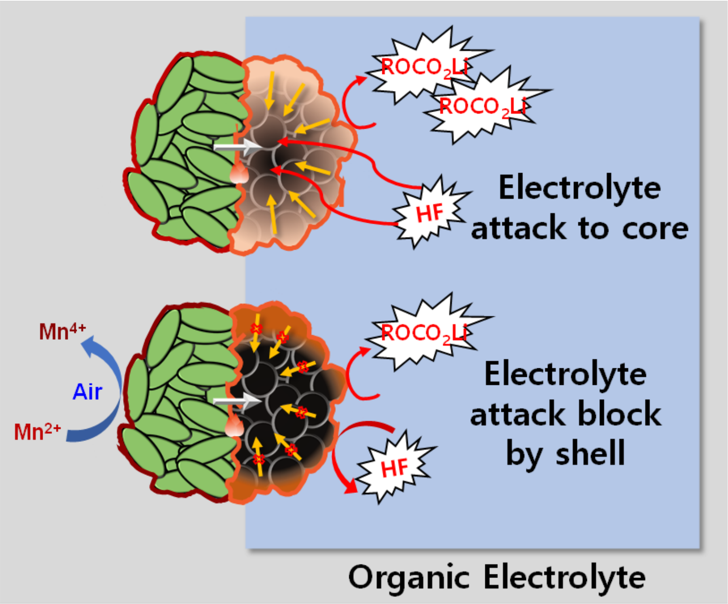
Chair: Seung-Ryong Kwon (Gyeongsang National University)

Suppressing Mn Diffusivity by Oxidation State Control for the Synthesis of Ni-Rich Core/Shell Structured Cathode Materials

Jin Ho Bang*, Jinha Shim[1]

Department of Chemical & Molecular Engineering, Hanyang University, Korea
[1]*Applied Chemistry, Hanyang University, Korea*

Cobalt’s rapid price increase, high toxicity, and limited reserves lead to its removal from the battery manufacturing industry. Structure-modified materials have been developed to reduce or eliminate Co without sacrificing battery performance. In particular, in the NiMn core-shell system, the Ni-rich core is responsible for high energy density, while the Mn-rich/Lower Ni shell serves to ensure interfacial stability and to promote high kinetic hindrance. However, in the coreshell structure, the Mn-rich shell-to-core interdiffusion leads to a higher exposure of Ni to the electrolyte at the surface, which can accelerate the electrochemical instability and capacity fading. Despite the current progress in various studies on mutual diffusion prevention, limitations such as reduction in initial capacity and increase in structural complexity still exist. In this work, we introduce a new simple method to prevent the interdiffusion of Mn. A simple surface oxidation treatment increases the valence state of Mn in the precursor and this higher valence Mn, which is chemically more stable, has a higher kinetic barrier for diffusion. This new methodology offers higher capacity retention and interfacial stability even with a small amount of Mn substitution.


$ROCO_2Li$
$ROCO_2Li$
HF
Electrolyte attack to core
Mn^{4+}
Air
Mn^{2+}
$ROCO_2Li$
Electrolyte attack block by shell
HF
Organic Electrolyte

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 10:00

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Solubility-enhancing hydrotrope electrolyte with tailor-made organic redox-active species for redox-enhanced electrochemical capacitors

JInhwan Byeon, Sukwon Hong[*], Seung Joon Yoo[1,*]

Department of Chemistry, Gwangju Institute of Science and Technology, Korea
[1]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

Redox-enhanced electrochemical capacitors (redox ECs) improve the energy density of conventional electric double-layer capacitors (EDLCs) via Faradaic reactions from redox molecules dissolved in the electrolyte. In such redox ECs, the solubility of redox compounds is a crucial factor that impacts cell performance. The most widely employed redox compounds, however, have low solubility in aqueous environment, thereby limiting further performance improvements. In the present research, we introduce the novel concept of a hydrotropic supporting electrolyte (HSE) that can serve as both an ion-conducting supporting electrolyte and a hydrotrope that enhances solubility. Using the HSE, the solubility of hydroquinone (HQ) increased 7-fold compared to that in the conventional aqueous sulfuric acid electrolyte. Based on this new insight, the dual-redox species triethanol-ammonium bromide-substituted anthraquinone (AQM-Br), which simultaneously serves as an anolyte and catholyte, was synthesized. Through mechanistic studies using the intermolecular nuclear Overhauser effect and dynamic light scattering, two different solubilization mechanisms, a co-solubilizer and the formation of a quasi-micelle structure were proposed based on how the structuring of the solute and hydrotrope changes. Using dual-redox-active AQM-Br, a redox EC was developed by adding p-TsOH as the HSE. This redox-EC produces a specific energy of ~58 Wh/kg at 0.5 A/g and retained 81% of its initial energy over 10,000 cycles at 5 A/g, with 99.2% coulombic efficiency. This in-depth investigation explains the chemistry of hydrotropic solubilization and offers design guidelines for the most effective use of hydrotropes for energy storage.

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 10:15

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Improved Stability of Peroxodicarbonate Dianions for Excellent Cyclability of CO2-Assisted Lithium–Oxygen Batteries at Low Temperatures

Jin-Hyuk Kang, Hye Ryung Byon[1,*]

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

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

Lithium-oxygen (Li-O2) cells suffer from various challenges including undesired reactions by the superoxide radical (O2•–) intermediate and high oxidation potential leading to the irreversible deposition of lithium carbonate (Li2CO3) on electrodes, resulting in rapid capacity fading from partial decomposition. Interestingly, by introducing CO2 gas, electrochemical and chemical routes in the Li-O2 cells can be altered to form a soluble peroxodicarbonate dianion (C2O62-), which significantly improves the reversibility of galvanostatic discharging and charging processes. The stability and molecular structure of C2O62– are influenced by temperature and aprotic solvents. A low temperature below 0 oC was necessary to maintain the stability of the C2O62-, in addition to utilizing an electrolyte solution with high ionic conductivity. Moreover, the molecular structures of C2O62- were affected by Li+ solvating powers of the solvents. We observed the anhydride-linked C2O62– in tetraglyme, but its poor ionic conductivity resulted in significant voltage polarization and capacity fading. On the other hand, DMAc, which offers better Li+ solvation, facilitated the formation of peroxo-linked C2O62– and provided sufficient ionic conductivity, even at a –10 oC. Our extensive study revealed that the Li–O2/CO2 (90/10 v/v%) cells exhibited the best cyclability with 0.5 M LiNO3/DMAc at –10 oC. During the cycles, the first charging plateau at 3.75 V (vs. Li/Li+), which is related to the C2O62- oxidation process, was elongated. Furthermore, the limited amount of Li2CO3 was fully decomposed during the second charging process, leading to no capacity fading over 100 cycles. Our positive results encourage us to develop future Li–O2/CO2 batteries and Li-air batteries with improved cyclability.

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 10:30

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Electrodeposited NiFe Nanoparticles on TiO_2 Nanotubes as an Efficient Oxygen Electrodes for Anion Exchange Membrane Electrolyzer

Shajahan Shaik, Jeonghyeon Kim[1], Sang-Il Choi[2,*]

Department of Chemisty, Kyungpook National University, Korea

[1]*Kyungpook National University, Korea*

[2]*Department of Chemistry, Kyungpook National University, Korea*

Designing effective and inexpensive electrodes with high electrocatalytic activity and excellent durability without using noble metal-based materials is a vital global challenge in hydrogen (H_2) production using electrochemical water splitting. An electrodeposition technique was used in the current work to prepare NiFe nanoparticles on TiO_2 nanotubes as an anodic electrode for anion exchange membrane water electrolysis (AEMWE). NiFe/ATNT electrode prepared under optimal conditions exhibited excellent electrocatalytic activity in a half-cell test with an overvoltage of 222 mV at 10 mA cm^{-2} for oxygen evolution reaction (OER) in 1.0 M KOH solution. The AEM water electrolyzer designed using NiFe/ATNT as an anode and Pt/C/ATNT as a cathode exhibited high cell performance of 1039 mA cm^{-2} at 1.8 V in 1.0 M KOH solution at 60 ^{o}C, which is better than electrolyzer performance of commercial Pt/C/CP // IrO_2/TF (665 mA cm^{-2}). It has also been reported that the electrolyzer performance could be upgraded by adjusting operating parameters during MEA preparation.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

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

Oral Presentation for Young Electrochemists

Room 205+206 THU 10:45

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Electrically Driven Selective Olefin Epoxidation by Co–TAML and Its Mechanistic Investigation

Suyeon Kim, Wonwoo Nam[1,*], Kyoungsuk Jin[2,*]

Department of Chemistry, Korea University, Korea
[1]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*
[2]*Chemistry Department, Korea University, Korea*

Epoxides are versatile chemical intermediates that are used in the manufacture of diverse industrial products. For decades, thermochemical conversion has been employed as the main synthetic route, but it has several drawbacks. Herein, we propose an alternative pathway, electrocatalytic epoxidation, using [Co^{III}(TAML)]$^-$ (TAML = tetraamido macrocyclic tetraanionic ligand) molecular catalysts. Under ambient conditions, the catalysts selectively epoxidized olefin substrates using water as the oxygen atom source, affording a broad scope for substrate oxidation. Electrokinetic studies shed further light on the mechanism of olefin epoxidation, which was found to involve rapid oxygen-transfer equilibrium followed by a rate-limiting electron transfer process. We verified that the use of a phosphate electrolyte successfully facilitated the Co$^{III/IV}$ redox process via the Libido rule, which may play a key role in the unprecedented high reactivity achieved by the [Co^{III}(TAML)]$^-$ catalysts.

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

New Trends in Chemistry Education

Room 204 FRI 09:00

Chair: Heesook Yoon (Kangwon National University)

An Analysis of Actual and Preferred Cases of Assessment in 'Scientific Inquiries in History' of Science Inquiry Experiment

Minhwan Kim, Taehee Noh[*]

Department of Chemistry Education, Seoul National University, Korea

In this study, we investigated actual cases of assessment science teachers conducted and the cases they preferred in a typical situation based on the curriculum in the context of 'Scientific Inquiries in the History' of Scientific Inquiry Experiment. A questionnaire composed of descriptive questions was developed and a survey was conducted with 70 science teachers with experience in teaching 'Scientific Inquiries in History'. Interviews were conducted with eight of them. The assessment cases were analyzed in terms of the assessment areas and assessment methods, and the results were compared. The analyses of the results revealed that 'scientific inquiry ability' accounted for the highest ratio of the assessment areas in the actual cases of assessment. There were few cases that assessed the core concepts presented in the curriculum, 'the nature of science' and 'scientists' inquiry methods'. The assessment methods were greatly biased toward the report method and various assessment methods were not used. In preferred cases of assessment, the ratio of cases that assessed the core concept increased slightly, however the frequencies remained at a low. As for the assessment methods in preferred cases of assessment, the measurement methods decreased, the performance methods increased, and the informal methods which were not shown in the actual cases appeared. However various assessment methods were still not used. Based on above results, plans to actively conduct NOS assessments in Scientific Inquiry Experiment are discussed. (This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea(NRF-2021S1A5A2A01061452))

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

New Trends in Chemistry Education

Room 204 FRI 09:20

Chair: Heesook Yoon (Kangwon National University)

The effects of semantic map reading strategies on the change in inference comprehension of high school students in science text reading

SuJin Lee, Jihun Park[1], Jeonghee Nam[1,*]

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

The purpose of this study is to investigate the effect of the semantic map reading strategy used in science text reading on the change in high school students' inferential comprehension as a sub-factor of reading ability. For this purpose, eight science text reading classes were conducted using semantic mapping reading strategy for 46 students in two science-focused classes in the third grade of high schools that were designated as science-focused schools located in small and medium-sized cities. In the analysis of changes in inferential comprehension, the statements of the answers written by students were classified into low, intermediate, and high levels using the analysis framework of inferential comprehension. For the classification of changes in inferential comprehension, the levels of the inferential comprehension was converted into scores. Accordingly, the average was compared and analyzed by giving 0 points for the low level, 1 point for the intermediate level, and 2 points for the high level. The correlation between students' inferential comprehension and science text reading ability was investigated, in order to find out what roles inferential comprehension plays in science text reading.

Oral Presentation : **EDU.O-3**
New Trends in Chemistry Education
Room 204 FRI 09:40
Chair: Heesook Yoon (Kangwon National University)

Analysis of Middle School Students' Interaction in Small Group Learning using Augmented Reality: Focusing on Dissolution and Solution Concepts

Nayoon Song, KiDoug Shin[1], Taehee Noh[1,*]

Center for Educational Research, Seoul National University, Korea
[1]*Department of Chemistry Education, Seoul National University, Korea*

This study analyzed paired middle school students' verbal and physical interactions in small group learning using augmented reality. Twelve 8th graders were paired to take classes of solubility and melting/boiling points based on augmented reality. These classes were videotaped and recorded. After the classes, all the students participated in a semi-structured interview. The results were analyzed in three sections; individual statement units of verbal interaction, interaction units of verbal interaction and physical interaction. In the individual statement units of verbal interaction, the proportion of information question/explanation was found to be high. In the interaction units of verbal interaction, the proportion of simple interaction was the highest, followed by elaborated interaction. Beneath the elaborate interaction, the proportion of cumulative interaction was found to be the highest, followed by reformative interaction. In the physical interaction, writing a worksheet and gazing at a virtual object were higher. On the basis of the results, effective ways to form a proper environment in small group learning using augmented reality are discussed.

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

New Trends in Chemistry Education

Room 204 FRI 10:10

Chair: Heesook Yoon (Kangwon National University)

Comparison of Level and Influencing Factors Academic Passion for Science PCK between Elementary School Pre-service and In-service Teachers

Hunsik Kang

Gifted Education, Seoul National University of Education, Korea

The purpose of this study is to compare th level and influencing factors of academic passion for science PCK between elementary pre-service and in-service teachers. In addition, a comparison between passion for science subject matter knowledge and passion for science pedagogical knowledge was made for each group of teachers. Participants were comprised of 182 students in college of education and 161 teachers. We analyzed between- and within-subject comparison for each component of academic passion for science PCK. Results of this study are as follows: First, between-subject comparison demonstrated that, in academic passion for science subject matter knowledge, in-service teachers had higher passion for ‘liking’ and ‘importance’ than per-service teachers, while pre-service teachers had higher passion for ‘time/energy investment’ than in-service teachers. In academic passion for science pedagogical knowledge, pre-service teachers had higher passion for ‘time/energy investment’ than in-service teachers. Second, within-subject comparison showed that only ‘harmonious passion’ was higher for science pedagogical knowledge than science subject matter knowledge in pre-service teachers. However, ‘liking’, ‘importance’, ‘time/energy investment’, and ‘obsessive passion’ were higher for science subject matter knowledge than science pedagogical knowledge in in-service teachers. The pre-service and in-service teachers selected some different factors that influenced their academic passion for science subject matter knowledge and science pedagogical knowledge. Educational implications are discussed.

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

New Trends in Chemistry Education

Room 204 FRI 10:30

Chair: Heesook Yoon (Kangwon National University)

Science Teachers' Perception of Artificial Intelligence Utilization Competency and Digital Competency for Advanced Scientific Inquiry Implementation

Mihyun Son

Division of Natural Sciences, Seoul National University, Korea

The purpose of this study was to find out the meaning of teachers' digital competency and AI utilization competency, and why such competencies are needed to carry out new scientific inquiries using rich data and artificial intelligence. To this end, leading teachers who actively carry out an advanced scientific inquiry in a new way were interviewed about teaching methods, motives, and perceptions of inquiry, and analyzed them. As a result of the study, science teachers needed these competencies for social and national needs, heightened crisis awareness according to changing student competencies, recognition of the need for changes in evaluation methods, and the use of tools for accurate concept learning. Also, the most important elements of the competency are convergent instructional design skills, an in-depth understanding of the basic principles of artificial intelligence, computer languages utilization skills such as block coding and text coding, and artificial intelligence platform utilization skill. This study can help establish the direction for fostering artificial intelligence competencies and digital competencies of science teachers.

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

General Session

Room 302 THU 09:00

Chair: Sungjun Bae (Konkuk University)

Microplastic distributions in a wastewater treatment plant in Korea: Removal efficiency, seasonal variation and effect of different treatment processes

Sang-Heon Na, EunJu Kim[1,*]

Division of Energy & Environment Technology, University of Science & Technology, Korea
[1]*Korea Institute of Science and Technology, Korea*

The necessity for plastic increases in line with the growth of industrialization, and the production of plastics is steadily increasing. However, 70% of plastics were wasted and some inadequate plastic waste management plastics disposed directly into the environment factor such as UV, rainfall, wind, and microorganisms. Inadequate plastic waste can be degraded to small particles from large particles by environmental factors. Plastic particles smaller than 5 mm, called microplastics (MPs), have been exposed to surface water such as rivers and lakes. Since the existence of MPs was first reported in 2005, many studies have been conducted in many fields as new micropollutants. This study assessed the seasonal and spatial distribution of MPs in wastewater treatment plants (WWTP). According to the characterization result, 114 ± 17 – 216 ± 65 particles/L for influent and from 0.26 ± 0.29 – 0.48 ± 0.11 particles/L for effluent. Meanwhile, quantitative analysis showed that 0.2% of MPs remained in the WWTP effluent although 99.8% of them have been successfully removed by the wastewater treatment process. These results highlight that WWTP is a main source of MPs in the surface water and long-term monitoring is required to accurate estimation of the MPs load from WWTPs.

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

General Session

Room 302 THU 09:20

Chair: Sungjun Bae (Konkuk University)

Sulfonated graphene based thin film composite membranes with simultaneous mitigation of silica scaling and organic fouling for brine treatment by pervaporation

Hasan Fareed, 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*

A novel tortuous brick and mortar structure utilizing intercalation of polyvinyl alcohol (PVA) on the sulfonated graphene oxide (SGO) membranes was specifically tailored for brine treatment by pervaporation to ensure excessive resistance to silica scaling and organic fouling as well as ultrafast water transport without compromising salt rejection. The synthesized SGO membrane showed a smoother surface morphology, improved zeta potential, and a higher hydration capacity than graphene oxide (GO) membrane. Further intercalation of PVA through glutaraldehyde (GA) crosslinking, confirmed by Fourier transform infrared spectroscopy and X-ray diffraction analysis, increased the cohesiveness of SGO-PVA-GA membrane and thus managed to withstand ultrasonication tests without any erosion of the coating layer. The pervaporative desalination test revealed that SGO-PVA-GA exhibits 62 kg m-2 h-1 of permeate flux with an extraordinary salt rejection of 99.99% for a 10 wt% NaCl feed solution at 65 °C. The 72 h-long organic fouling, silica scaling, and combined fouling and scaling tests proved that the SGO-PVA-GA membrane sustains a stable flux with less scaling and fouling than the GO-PVA-GA, attributable to dense surface negative charges and great hydration capacities caused by sulfonic acid. To conclude, the SGO-PVA-GA membrane carries superlative advantages for long-term brine treatment by pervaporation related to its ability to withstand silica scaling and organic fouling.

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

General Session

Room 302 THU 09:40

Chair: Sungjun Bae (Konkuk University)

Ni-based electrocatalytic desalination with bipolar membranes for concurrent acid and base production

Byeong-ju Kim, Hyunwoong Park*

School of Energy Engineering, Kyungpook National University, Korea

Bipolar membranes have been used in a variety of fields to electrochemically dissociate water molecules into H+ and OH- and consequently modulate the pH of electrolyte without adding chemicals. Here, we developed an electrocatalytic desalination device with bipolar membranes producing acid (HCl) and base (NaOH), whose anion (Cl-) and cation (Na+) is transported from saline water via an anion exchange membrane (AEM) and a cation exchange membrane (CEM), respectively. Simply one-step-electrodeposited NiFe-LDH and NiMo on the Ni foam substrate were connected as the anode and the cathode, respectively, which showed low overpotentials comparable to noble metal electrodes. Due to continuous water dissociation at the BPMs, the anolyte (1 M KOH) and catholyte (1 M H2SO4) pH was steadily maintained in their initial values and favorable to oxygen and hydrogen evolution reactions with the Faradaic efficiencies of >90%. Stacked with the AEM/CEM array, the device was able to desalinate faster and more efficient than the single array at the specific energy consumption of 1.8 kWh m-3. Possible pH-swing application of saline water carbon capture was also discussed.

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

General Session

Room 302 THU 10:00

Chair: Sungjun Bae (Konkuk University)

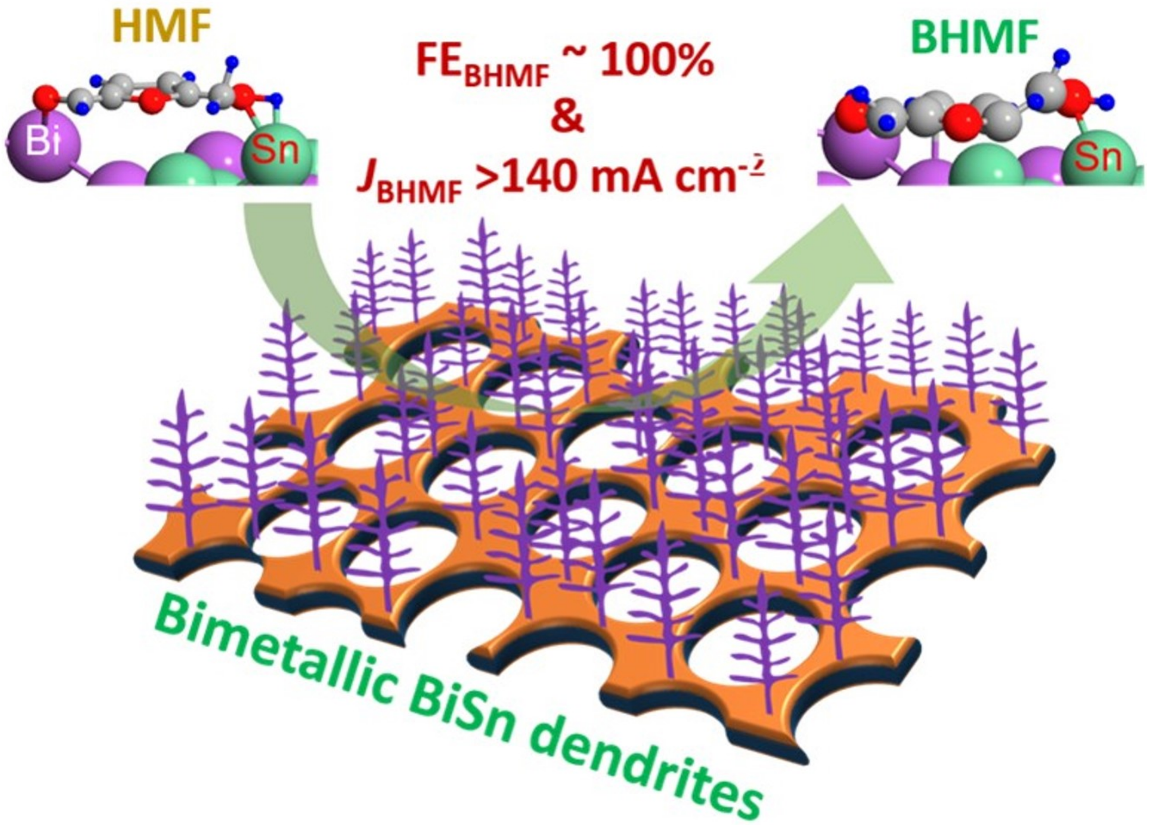
Highly selective electrochemical hydrogenation of 5-Hydroxymethylfurfural to 2,5-Bis(hydroxymethyl)furan on porous dendritic BiSn electrode

Guangxia Piao[*], **Hyunwoong Park**[*]

School of Energy Engineering, Kyungpook National University, Korea

Electrocatalytic hydrogenation of 5-hydroxymethylfurfural (HMF) to 2,5-bis(hydroxymethyl)-furan (BHMF) opens an alternative route to conventional heterogeneous catalysis with H2 at high temperature and pressure. This study synthesizes porous dendritic Bi, Sn, and BiSn electrodes using an in-situ generated hydrogen bubble template to evaluate their electro-catalytic activity toward HMF conversion to BHMF. DFT computations on adsorption energy (Eads) and elementary hydrogenation reaction steps of HMF predict the superiority of Bi to Sn, as well as the intermediate behavior of BiSn between Bi and Sn. The pH affects the competing process of hydrogen evolution reaction (HER) and the distribution of the products derived from HMF reduction. The dendritic BiSn catalyst generates a current density of -145.7 mA cm-2 at Faradaic efficiency (FE) of ~100% for BHMF production at pH ~7 (corresponding to the BHMF production rate of ~2.7 mmol h-1 cm-2) in prolonged electrolysis. The BiSn cathode is further demonstrated to drive HMF hydrogenation at FE of ~100% when coupled to NiOOH anode for HMF oxidation to 2,5-furandicarboxylic acid at FE of ~95%. Considering the material cost (〈5% of Ag price) and quick synthesis (〈40 s), dendric BiSn can be considered as a potential candidate for HMF hydrogenation.

This research was supported by the National Research Foundation of Korea (NRF-2021K1A4A7A02102598).


HMF
FE_BHMF ~ 100%
&
J_BHMF >140 mA cm^-2
BHMF
Bi
Sn
Sn
Bimetallic BiSn dendrites

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

General Session

Room 302 THU 10:20

Chair: Sungjun Bae (Konkuk University)

Recovery of Palladium from electronic waste for selective oxygen reduction reaction

Kyuri Cho, Wooyul Kim[1,*]

Korea Institute of Energy Technology, Korea
[1]*Department of Energy Engineering, Korea Institute of Energy Technology (KENTECH), Korea*

The oxygen reduction reaction (ORR) is considered as an promising source for supplying energy alternatively. ORR can be driven in two ways, two-electron ORR and four-electron ORR. The former transfers oxygen to a favorable green oxidant, hydrogen peroxide (H_2O_2). Thus, the two-electron ORR is being increasingly investigated and evolved in various ways. However, the conventional anthraquinone process for the two-electron ORR has some disadvantages, such as the cost problems of precious metals, byproducts issues, and also the complicated processes. Thus, making catalyst by electrodepositing metal particles as a single atom from e-waste would shed a light to overcome those problems. Here, we precisely controlled spatially well-dispersed Palladium catalysts on mildly reduced Graphene Oxide (mrGO) by simple electrochemical e-waste recovering method. The as-prepared Pd-mrGO electrocatalysts were applied for oxygen reduction reactions to produce H_2O_2. More details will be addressed in the poster.

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

General Session

Room 302 THU 10:40

Chair: Sungjun Bae (Konkuk University)

Stand-alone simultaneous drive system for electrocatalytic arsenite oxidation combined with CO_2 reduction to formate

Wonjung Choi, Yiseul Park, Hyunwoong Park[1,*]

Pukyong National University, Korea

[1]*School of Energy Engineering, Kyungpook National University, Korea*

In this research, a stand-alone simultaneous drive system for electrocatalytic arsenite oxidation combined with CO_2 reduction to formate was reported. The electrocatalytic CO_2 reduction reactions (CO_2RRs) to produce the formate in a circum-neutral bicarbonate solution were performed on Bi nanoparticle electrodeposited on a Ti plate and it showed a high Faradaic efficiency (FE) of ~100%. Bicarbonate solution is a suitable electrolyte for CO_2RRs, but not for As(III) oxidation. The FEs of As(III) oxidation were reduced due to an unfavorable electrolyte and competition with the oxidation of water; however, reactive chlorine species (RCSs), produced by chloride oxidation, could be doubled enhanced the FEs of As(III) oxidaiton. The overall redox system was developed to focus on simultaneously driving the half-reactions optimized under different conditions without degrading performance relative to half-reactions. In the final step, a stand-alone PV-electrolysis hybrid system operated without an external power source was developed through the combination of Photovoltaic cells and electrolysis system. In order for the PV-electrolysis hybrid system to operate optimally, the PV cell specifications were chosen to correspond with the experimental conditions and power requirements of the electrolysis system. As a result, the 〉10% solar-to-system conversion efficiencies were achieved for the PV-electrolysis hybrid system, and the FEs of the redox reactions were attained in the same optimal results as driven by an external power source.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Facile Approach to Synthesis of Ionic Polymers and Copolymerization of Immiscible Monomers Using Ball-milling

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

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

The synthesis of ionic polymers, which can be applied to various fields such as batteries, drug delivery, hydrogels, and ion filters, has been realized under a solid-state mechanochemical ball-milling manner, promoting an eco-friendly and straightforward synthetic process. The conventional solution polymerization of ionic monomers has suffered a narrow choice of solvents and poor efficiency; direct ball-milling polymerization is not limited by solubility and miscibility. This work includes free-radical polymerization of styrene and (meth)acrylic ionic monomers and Ru-initiated ring-opening metathesis polymerization of norbornenyl ionic monomers, proving the excellent performance of mechanochemistry producing desired product polymers under the ball milling from a wide range of ionic monomers. Further exploration was accomplished with mechanochemical copolymerization of immiscible monomer pairs (ionic/hydrophobic) including sodium acetate/pyrene and sulfobetaine/porphyrin moiety. This approach facilitates the production of ionic polymers without purifications in a short time.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Characterization of Self-healing Network Ionic Polymers Based on Piperazinium Cross-linker

Jongchan Shin, Minjae Lee[1,*]

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

Ionic polymer-based electrolytes can replace conventional lithium-ion battery liquid electrolytes due to their high ion conductivity. They can resolve the problems of liquid electrolyte's flammability and leakage. In this study, network ionic polymers were synthesized using piperazinium-Tf_2N cross-linker and co-monomers. This new synthesized self-healing network ionic polymers exhibit good self-healing properties; cutting surface is recovered within 1 hour at 80 ^oC. Self-healing properties is still maintained for the polymer composites with 10 wt% of Li salt. They exhibit comparable ionic conductivity of 4.53 $x10^{-6}$ S/cm at 50 ^oC. These self-healing network ionic polymers can produce a flexible film at room temperature. Electrochemical stability is also superior: they are stable up to 6.0 V (vs. Li/Li^+). The detailed structures and properties of these materials will be discussed in the presentation.

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Poster Presentation : **POLY.P-3**
Polymer Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Excellent Carrier Mobility and Low Voltage Operation in Organic Transistors Using Six-Branched Organic Azide with Ultrahigh Crosslinking Efficiency

MyeongJae Lee, BongSoo Kim[1,*]

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

Polymer gate dielectric is an essential component in organic thin film transistors (OTFTs). To achieve OTFT on an industrial level, requirements such as high carrier mobility, enabling low manufacturing voltages, compatibility with reliable high-resolution patterning processes, and high technical and electrical stability must be fulfilled. Herein, we show a facile strategy for forming a polymer gate dielectric and polymer seimiconductor by using a newly designed and synthesized organic azide-based crosslinker (6Bx). The 6Bx crosslinker consists of six organic azide moieties, which permits the photo-crosslinking in host polymers and the generation of a high-resolution-patterned polymer gate dielectric with a reduced leakage current (7 × 10-9 A cm-2 at 1 MV cm-1). Moreover, the utillization of 6Bx crosslinker facilitates the realization of low-voltage OTFT operation (< 3 V) and excellent and stable OTFT device operation. Futhermore, p- and n-type polymer OTFTs employing photo-crosslinked PMMA gate dielectric material indicated high carrier mobilities of 12.42 and 10.11 cm2 V-1s-1 at < 3 V, respectively, which are remarkably improved carrier mobilities at low voltages operation compared to those by conventional materials. The presented concept of high efficiency crosslinker will open a avenue in developing solution-processable, easily patternable OTFTs for next-generation flexible & wearable electronic devices.

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

Polymer Chemistry

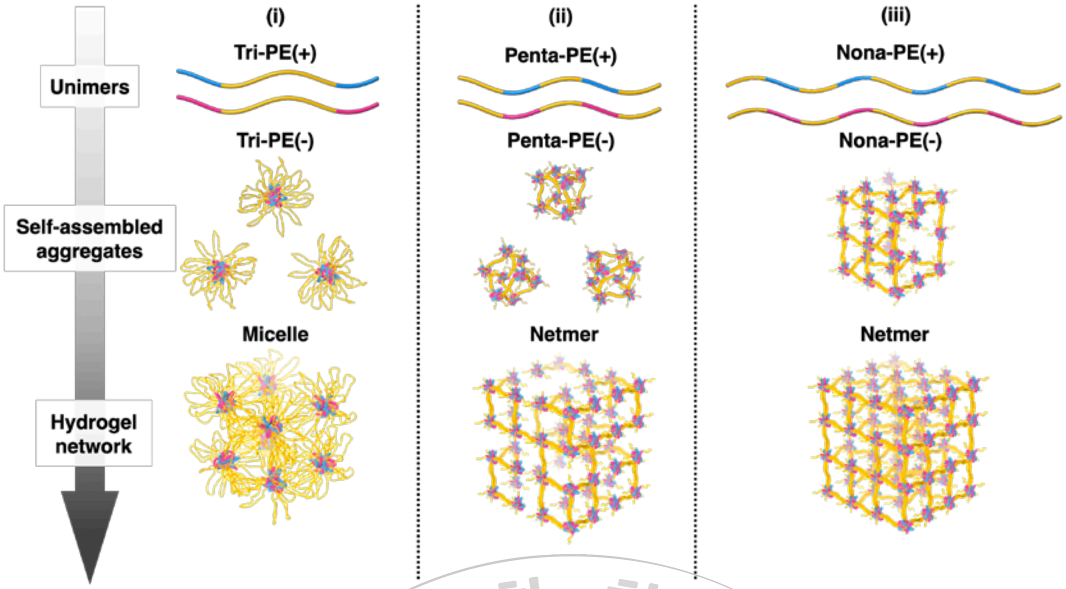
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Bridge-rich and loop-less hydrogel networks through suppressed micellization of multiblock polyelectrolytes

Jihoon Han, Younsoo Kim*

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.



Unimers
Self-assembled aggregates
Hydrogel network
(i)
Tri-PE(+)
Tri-PE(-)
Micelle
(ii)
Penta-PE(+)
Penta-PE(-)
Netmer
(iii)
Nona-PE(+)
Nona-PE(-)
Netmer

Poster Presentation : **POLY.P-5**
Polymer Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Side-Chain Engineered p or n-Type Nonaqueous Polymeric Ionic Gels for Sustainable Thermoelectric Energy Generators

Sungryong Kim, Taehyun Kim[1], Taiho Park[1,*]

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

Herein, we synthesized the p-, and n-type polymer ion gels (PIGs) which are composed of hydrophobic polymers with long ionic side chains and bulky mobile ions. The ionic side chain could realize that single type ions (cation or anion) diffuse selectively and prevent the phase separation between ionic side chains and mobile ions under thermal stress. Bulky mobile ions are used not only as charge carriers for ionic conductivity, but also plasticizer to lower the Tg of polymers. Its enable that our PIGs with 75% ion moieties exhibit highly stretchable (811% in p-type and 833% in n-type, respectively) and self-healing properties (99% self-healing ability within 1h) under ambient condition (RH 30%). In addition, the methyl acrylate backbone in random copolymer as well as bulky mobile ions hardly absorb the water from the environment due to their low hygroscopic properties and induce the entanglement in polymer network. This enable fast saturation (3rd cycle) in repeated stretching test, which realize stable mechanical property of polymers. In a result, our PIGs exhibit highly stretchable, self-healable, thermal, and mechanical stabilities. We fabricate a p-, and n–type PIGs-based thermoelectric energy generator (TEG) with operability at ambient condition (RH 30%), thermal stability, stretchability, and self-healing properties. The TEGs maintain their initial performance under various deformations and thermal stress. In addition, their ionic conductivity and Seebeck coefficient are consistent under 50% strain (67% and 95%, respectively), several self-healing (100% and 99%) and after 5days (100% and 99%). The TEGs with novel PIGs open up the stretchable electronics with high self healing properties irrespective of humidity condition.

Poster Presentation : **POLY.P-6**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Polymerization-Induced Microphase separation in Janus Bottlebrush Polymers

Changsu Yoo, Myungeun Seo*

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

Polymerization-Induced Microphase separation (PIMS) has been used for generating bicontinuous polymeric nanomaterials. The polymerization of the second block results in increase of segregation strength, yielding microphase separation and multifunction monomer capture of the morphology before the order to disorder transition. However, achieving long-range ordered nanostructure is indispensable for block copolymer-based nanopatterning. But PIMS without multifunctional monomers suffers several problems like the mechanical property, homogeneity, and batch-to-batch difference. Here, we explore the effect of Janus bottlebrush polymer architecture on PIMS without a crosslinker system. Bottlebrush polymers, which have densely grafted side chains, show extended morphologies. The preorganization of different side chains on the Janus bottlebrush backbone exhibits efficient self-assembly compare to their linear counterpart. The synthetic pathway and microphase separation behavior of both linear and Janus bottlebrush polymer will be discussed in detail.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

[Withdrawal] Reversible Phase Transition of Polymerization-Induced Self-Assembly by Switching Polymerization/Depolymerization Equilibrium

Jiyun Nam, Myungeun Seo*

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

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of the Robust Ion-exchangeable Nanoporous Separator by Polymerization-induced Microphase Separation for Lithium Metal Battery Application

Taeseok Oh, Hye Ryung Byon, Myungeun Seo*

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

Lithium Metal Battery is one of the most attractive batteries nowadays because of their high energy density. Like other batteries, lithium metal batteries also require a separator that physically separates two electrodes and facilitates the conduction of lithium ions. However, conventional commercial separators such as Celgard do not exhibit permselectivity and not showing controlled transport due to the macropores. This uncontrolled transport disrupts the solid-electrolyte interfaces and reduces cell performance and lifetime. Here, we ail that nanoporous polymers with 3D continuous structures with controlled pore size and surface tailorability can be strong candidates as permselective membranes. In this study, we synthesized a porous polymer by adjusting the crosslinking density and pore size in Polymerization-induced microphase separation and measured the thermal and chemical stability and ion conductivity. The nanoporous polymer membrane we synthesized is stable in organic solvents, and can effectively induce polarization of lithium ions and anions by controlling surface charge through sulfonation. In addition, by controlling the pore size, the effect of the pore size of the polymer on the conductivity was analyzed and the pore size was optimized. Through this study, we will synthesize a nanoporous polymer for lithium metal batteries that surpasses commercial separators and apply it to actual cells.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Structure and Behavior of triblock-type amphiphilic random copolymers with terminal styrene blocks

Jimin Yoo, Myungeun Seo*

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

It has been reported that amphiphilic random copolymers with hydrophobic and hydrophilic repeating units form a bilayer-folded lamellar mesophase(Lf) containing periodic folding structures in water because local curvature mismatch is caused by local heterogeneity of sequences. We introduced styrene triblock copolymers with amphiphilic random copolymers as the middle block. This copolymer forms polystyrene domains in water and maintains the folding structure, which is expected to observe the folding-unfolding structure when the external force is applied. We used reversible addition–fragmentation chain transfer (RAFT) polymerization to obtain polystyrene of different lengths on bifunctional CTA and synthesize amphiphilic copolymers with the degree of polymerization under conditions forming a bilayer-folded lamellar structure. The structure of the triblock copolymer was analyzed by small-angle X-ray scattering (SAXS) measurement after hydrogels were made with concentrations forming the Lf phase reported in previous studies.

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Divergent Chiral Amplification Results from Self-Assembly between Hierarchies under Kinetic Control

Jun Su Kang, Kangseok Kim, Myungeun Seo*

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

Homochirality in life on Earth plays a crucial role in creating various biological structures and functions, which are closely related to the evolutionary process. Such a chiral environment is considered a result of the transfer and amplification of chirality encoded in prebiotic molecules during the hierarchical self-assembly across multiple length scales. While there are many reports that deal with chiral communications between molecular levels in molecular self-assembly or polymeric chain systems under thermodynamic control, only a few cases have studied chiral interaction between hierarchies beyond the molecular scale. Here, we explore the development of supramolecular chirality under kinetic control by using chiral and achiral triarylamine (TAA) derivatives that can be hierarchically self-assembled. By using temperature-dependent measurements, we track the diverse expressions of supramolecular chirality caused by the interplay between helices. We will discuss how the complex assembly pathway affected the resulting supramolecular structures and helicities in the evolutionary process.

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

Polymer Chemistry

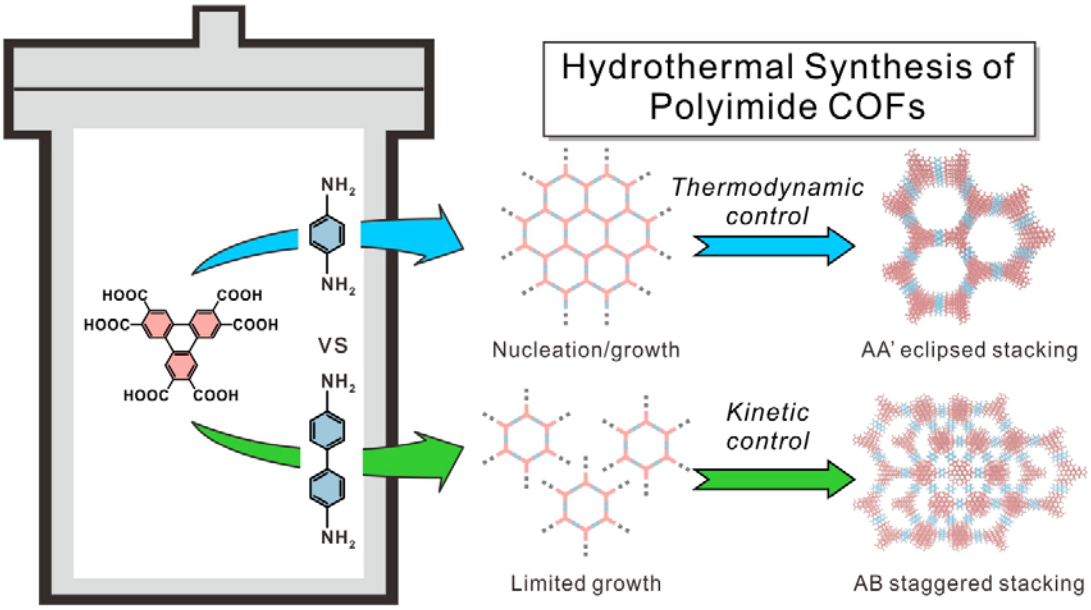
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks

Taehyung Kim, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

Despite its abundance, water is not widely used as a medium for organic reactions. However, under geothermal conditions, water exhibits unique physicochemical properties, such as viscosity, dielectric constant, and ionic product become similar to those of common organic solvents. In this study, for the first time, we synthesized highly crystalline polyimide-based covalent organic frameworks (PICs) under geomimetic hydrothermal conditions. By exploiting triphenylene-2,3,6,7,10,11-hexacarboxylic acid in combination with various aromatic diamines, PICs with various pore dimensions and crystallinities were synthesized. XRD, FT-IR, and DFT calculations revealed that the solubility of the oligomeric intermediates under hydrothermal conditions affected the stacking structures of the crystalline PICs. Furthermore, the synthesized PIC demonstrate promising potential as an anode material in lithium-ion battery owing to its unique redox-active property and high surface area.


Hydrothermal Synthesis of Polyimide COFs
NH2
NH2
HOOC
COOH
HOOC
COOH
HOOC
COOH
VS
NH2
NH2
Thermodynamic control
Nucleation/growth
AA' eclipsed stacking
Kinetic control
Limited growth
AB staggered stacking

Poster Presentation : **POLY.P-12**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ion-induced macroscopic morphological transformation of poly(ethylene glycol)-b-poly(styrene) (PEG-b-PS) by modulating the salting-out effect and cation matching effect

Valene Wang, Kyoung Taek Kim*

Division of Chemistry, Seoul National University, Korea

The modulation of morphologies of soft nanostructures formed by the solution self-assembly of block copolymers is of significance for a spectrum of applications. In particular, non-synthetic pathways to induce morphological transformation of the block copolymer have been of utmost interest because of the ability to achieve desired morphologies with minimal laborious synthesis. Herein, we report the synthesis of amphiphilic block copolymers composed of tri-arm linear, conventional linear and crown ether end-functionalized hydrophilic polyethylene glycol (PEG) blocks, and hydrophobic polystyrene (PS) blocks. The addition of lithium ions resulted in different extents of salting-out effect in different BCPs due to the architecture and the end-group functionalized hydrophilic segments as the decisive factors. Furthermore, the host-guest recognition between 12-crown-4 ether and lithium cation contributes significantly to the morphological transformation of the polymer vesicles to polymer cubosomes.

Poster Presentation : **POLY.P-13**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Poly[(1,1-disubstituted-3,4-diphenyl-2,5-silolene)-co-(ethynylene)] and Electrochemical Properties

Ji hun Lee, Young Tae Park[1,*]

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

Disubstituted(R = *iso*-Pr, *n*-Hex, Ph)-bis(phenylethynyl)-silanes were reacted with lithium naphthalenide, anhydrous zinc chloride, and *N*-bromosuccinimide (NBS) to obtain 1,1-disubstituted(R = *iso*-Pr, *n*-Hex, Ph)-2,5-dibromo-3,4-diphenyl-siloles, respectively. Poly[(1,1-disubstituted(R = *iso*-Pr, *n*-Hex, Ph)-3,4-diphenyl-2,5-silolene)-co-(ethynylene)], which are conjugated polymers containing with silolene and acetylene, were synthesized through the Stille coupling reaction of 1,1-disubstituted(R = *iso*-Pr, *n*-Hex, Ph)-2,5-dibromo-3,4-diphenyl-siloles and bis(tributylstannyl)acetylene as co-monomers, respectively 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, FT-IR, TGA, GPC and UV-vis spectroscopy. The bend gaps of the polymers were analyzed through a Gaussian program. The electrochemical properties of the prepared polymers as anode materials for lithium-ion batteries was also studied.Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Molecular Structural Changes Affecting the Self-Assembly Process of Triarylamine-based Supramolecular Polymers

Kangseok Kim, Jun Su Kang, Myungeun Seo*

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

Numerous studies are being conducted to determine the source of life. One approach is to investigate the origin of the preference for single-handed structures in amino acids and proteins, known as homochirality of biomolecules. Circularly polarized light (CPL), which is believed to originate from extraterrestrial sources such as supernova explosions, can cause the observed enantiophobic behavior by photochemical interaction with matter on the Earth's surface. This transfer of chirality from photons to matter can create asymmetry at the molecular level and lead to chiral supramolecular systems with useful chiroptic properties. Recent research is focused on the self-assembly through the interaction of C3-symmetric molecules containing a triarylamine (TAA) core and CPL. When a diacetylene (DA) group is incorporated into the side chain of these molecules, the resulting supramolecular helicity can be controlled in a chlorinated solvent.1,2 These structures exhibit high circular dichroism values, indicating their promising chiroptic properties. Here, we aim to observe the effects of structural manipulation on the self-assembly process and to identify the organic contributions of these molecules in creating supramolecular polymers. The outcome of this work is expected to facilitate the creation of molecules with high g-value by developing a molecular library.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Metal-imprinted Polymer Hydrogel based on colorimetric Azo-Quinolinol for selective detection and separation of Cobalt(II) ions from aqueous solutions.

Soyoung Park, Hyung-il Lee*

Department of Chemistry, University of Ulsan, Korea

We propose a technique for simultaneous detection and separation of cobalt established in a selective coordination-based colorimetric probe in Metal Imprinted Polymer Hydrogel (MIG). Especially, the N,N'-dimethylacrylamide (DMA), (E)-2-((4-(Diazenyl(8-hydroxyquinolin-5-yl))phenyl)(methyl)amino)ethylacrylate (M1) are copolymerized by free radical copolymerization to yield the polymeric probe [p(DMA-co-M1] (designated as P1). M1 contains a selective 1:1 Co(II) binding site. P1 exhibited a sensitive and selective colorimetric response to Co(II) in aqueous media that could be detected with the naked eye through a yellow to red color change. The separation behavior in that MIG was evaluated with Hydrogel (HG), demonstrating a better MIG response to Co(II) separation and the success of imprinting. The selective separation of Co(II) in presence of an approximately 10-fold excess of Fe(II) ion present in excess, was studied. The selectivity of MIG has been modified through metal ion imprinting technique for its potential application of radioactive waste in nuclear industry.

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

Polymer Chemistry

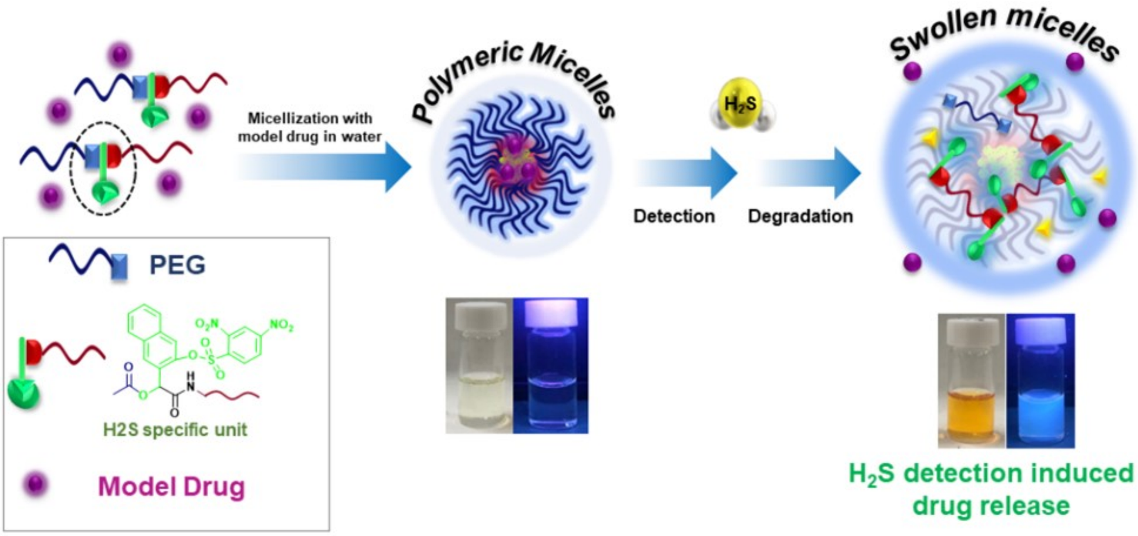
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Hydrogen Sulfide Detection Induced Burst Release of Model Drug from Polymeric Micelles

Nabilah Firyal Suhendra, Hyung-il Lee*

Department of Chemistry, University of Ulsan, Korea

Passerini multicomponent polymerization (PMCP) is simple and uncomplicated polymerization which can produce complex soft materials in a single pot using well-defined, structurally diverse polymers. These materials, which have been reduced to nanoscale dimensions, can now be used to develop so-called smart drug delivery systems, thereby allowing the safe administration of medicinal drugs to specified regions. In this study, a poly(ester-amide)-based amphiphilic polymer (named P1) is prepared for the burst release of a model drug, rhodamine, from polymeric micelles, triggered by hydrogen sulfide (H2S) detection. P1 was synthesized by the Passerini multicomponent polymerization of a hydrophobic H2S-specific unit (M1) with 6-isocyanohexanoic acid, and hydrophilic polyethylene glycol (PEG) dicarboxylic acid. When P1 self-assembles in water, it generates polymeric micelles consisting of a hydrophilic PEG shell and a hydrophobic core derived from M1 with 6-isocyanohexanoic acid. P1 micelles exhibited selective colorimetric (colorless to yellow) and fluorometric (non-emissive to blue emission) H2S detection in water. The limit of detection was as low as 0.09 mM. Upon the exposure of H2S to a P1 micelle solution encapsulating the hydrophobic model drug, rhodamine, H2S detection induced a sequential and self-destructive elimination process of the polymer backbone, resulting in the swelling of the micelles and the abrupt release of rhodamine.


Micellization with
model drug in water
Polymeric Micelles
H_2S
Detection
Degradation
Swollen micelles
PEG
O_2N
NO_2
H2S specific unit
Model Drug
H_2S detection induced
drug release

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Ion Gel Reinforced by Surface-Modified Aramid Nanofiber (ANF)

Seonwoo Yang, Taeseok Oh[1], Myungeun Seo[1,*]

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

Ionic liquids (IL) show unique features of low volatility, nonflammability, electrochemical stability, and high ionic conductivity. There are many fields where ILs can be applied, such as electrochemical actuators, supercapacitors, or lithium ion batteries. However, ILs are “liquid”, which means that it cannot maintain its form. To utilize ILs in actual necessary fields, mechanical strength enough to maintain its shape is required. Ion gels were reported with triblock copolymers composed with IL-phobic hard domain and IL-philic soft domain. These gels showed phase-separated behavior and enhanced mechanical strength, albeit lowered ionic conductivity. In our work, aramid nanofiber filler was utilized to enhance mechanical strength with minimal loss of ion conductivity. Physical properties and electrochemical characteristics were examined with respect to filler loading.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Metal-Chelated Polyphenol Complexes for Functional Composite Materials

Sang-Min Lee

Department of Chemistry, The Catholic University of Korea, Korea

Tannic acid (TA) as a natural polyphenol has been exploited as a multivalent cross-linker for polymer networkformation due to its excellent adhesion property, arising from multiple noncovalent chemical interactions. Additionally, the highly extensive coordination generality of TA for versatile metal cations allows for the biocompatible passivation of solid substrates and colloidal particles by facile metal−organic complex formation. In this presentation, we demonstrate that the excellent coordination property of TA enables the immobilization of versatile metal cations at the internal polymer networks, showing the great potential of metal-chelated TA composite as a biofunctional component for further applications.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A Structural Strategy for Stable Quinoidal Conjugated Polymer: Incorporation of Strong Acceptor

Younghyo Kim, Jeongjin Hong, Yerin Lee, Dong-Yu Kim*

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

Conjugated polymers have been extensively researched for various electronic devices because of their superior charge transport properties arising from π-orbital overlap. In particular, quinoidal conjugated polymers exhibit unique properties, such as high co-planarity, narrow bandgap, and open-shell diradical characters that are often not accessible in aromatic conjugated polymers, making them promising for a wide range of applications. Although diverse molecular design strategies for quinoidal conjugated polymers have been proposed to modulate their intriguing features, almost all the reported quinoidal conjugated polymers have limited structures consisting of quinoidal units and simple donor counterparts. For this reason, most quinoidal conjugated polymers are supposed to have stability issues, which was attributed to their high-lying HOMO energy level.In this research, a stable quinoidal conjugated polymer incorporating a strong acceptor unit was designed and synthesized for a lower energy level. Previously reported quinoid unit, AzaQuBT was copolymerized with the acceptor unit. The polymer is expected to exhibit enhanced stability due to its low HOMO energy level, resulting in the stabilization of open-shell diradicals. Consequently, this structural strategy for quinoidal conjugated polymer will provide great advantages for applications in organic devices.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Layer-by-Layer Assembled Nanofibers for Sequential and On-Demand Drug Delivery Platform

Sunyoung Yun, Baljinder Singh, Myoung-Hwan Park[1,*]

Department of Convergence Science, Sahmyook University, Korea
[1]*Department of Chemistry, Sahmyook University, Korea*

Sequential release-based drug delivery systems (DDS), which often rely on a variety of micro- or nanocarriers, may hold the key to treating many diseases. In this study, we investigated layer-by-layer assembled nanofiber platforms loaded with two drugs, camptothecin (CPT), encapsulated in nanofibers and doxorubicin (DOX) in the layers. Gold nanorods with near-infrared absorbance were inserted into the nanofibers to produce localized heat by plasmon resonance when exposed to light. As a result, the thermally responsive polymer can shrink and swell for controlled drug release. Linear-polyethylenimine (LPEI), a polycation, is used as a first layer and poly(sodium 4-styrenesulfonate) (PSS), a polyanion, is used as simply compensated the positive surface charge of the previous layer. Positively charged DOX was introduced in the layers. Initially, DOX was released to a lesser extent at pH 7.4 and showed a higher released amount at pH 6. Thereafter, the CPT was released in a controlled manner upon NIR irradiation. This study provides a flexible framework for regulated and safe drug delivery in specific areas and can be used to treat various topical diseases.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

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

Jaewon Choi, Taehun Chung[1], Ryo Yoshida[2], Younsoo Kim[1,*]

Pohang University of Science and Technology, Korea
[1]*Department of Materials Science and Engineering, Pohang University of Science and Technology, Korea*
[2]*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, for the overall mechanical oscillation of the gel, the size of the gel must be smaller than a chemical wave of several hundred micrometers. Furthermore, the BZ reaction required strong acidic conditions, and the duration of this reaction was short. These problems could be overcome by using specific hydrated protic ionic liquids (PILs) as an alternative medium for the BZ reaction. However, no oscillation was observed in conventional self-oscillating gels because of the low diffusivity of the BZ substrates into the gels in the highly viscous solution, such as hydrated PILs.Herein, we designed novel self-oscillating gels showing fast and large deformation by tuning the internal structure of the gels. Using the collapsed form of poly(N-isopropylacrylamide) in a salt solution, it is possible to synthesize the phase-separated structures showing fast and large shrinkage of the gels. We prepared the poly(NIPAAm-co-Ru(bpy)3) gel with the phase-separated structures, and it was immersed in a catalyst-free BZ solution. Interestingly, our phase-separated gels can oscillate even in a highly viscous solution owing to its high diffusivity. Furthermore, our gel exhibited a fast propagation rate and long wavelength of the chemical wave. As a result, even in centimeter-scale bulk gels, overall swelling/de-swelling oscillations could be exhibited, an unprecedented oscillation that significantly improved the dimension of oscillations.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Deuterated NHC Carben Ir(III) Complexes for the Solution- and Vacuum-Processed Deep-Blue Phosphorescent Organic Light-Emitting Diodes

Kim Hyerin, Sung-Ho Jin[1,*], Yeong Soon Gal[2,*], Jieun Lee

Pusan National University, Korea
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[2]*Department of Fire Safety, Kyungil University, Korea*

Organic Light Emitting (OLED) have focused on developing stability, efficiency and lifetime for next-generation phosphorescent OLED (PHOLED). Herein, we designed and synthesized a new Ir(III) NHC complexes with replace the hydrogen to deuterium compounds, mer-Ir(D7)3 which exhibited bright, deep-blue emission, with emission maximum between 450 and 460 nm. In this study, mer-tris-(N-D5-phenyl, N-D2-benzyl-pyridoimidazol-2-yl)iridium(III) (mer-Ir(D7)3) as dopant, TSPO1 and TPBi as host exhibited high efficiency of 19.2% CIE(x, y) coordinates of (0.148, 0.112) and maximum brightness (Lmax) of 21311 cd m-2, by device 2 with a 50 vol% doping ratio. The result findings, the deuteraion of Ir(III) complex is a promising candidate for reducing power consumption in display applications.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Sequencing of high-molecular weight uniform macromolecules by sequence-specific cleavage

HeeJeong Jang, Hyunseon Chu, Hyo Joo Noh, Kyoung Taek Kim[1,*]

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

Data is exponentially increasing due to online life patterns changed by COVID-19. For storing a large amount of data, conventional technologies including magnetic, optical, and electronic media have limitations such as low information storage density and loss of information. DNA and synthetic polymer have evolved as alternative of data storage. In synthetic polymer, sequence-defined polymer is synthesized to proceed with encoding of information. In many cases, decoding the information stored in sequence-defined polymers rely on tandem mass spectrometry, which occurs the fragmentation of the parent molecules. However, large molecular weights (>10 kDa) cannot be sequenced by tandem mass spectrometry due to limitation of instrument. Here, we attempt to overcome this limitation by synthesizing large molecular weight sequence-defined poly(phenyllactic-co-lactic-co-mandelic acid)s (PcLcM). The mandelic acid of PcLcM causes cleavage at specific sites on the polymer backbone through hydrogenation. These fragments are sufficiently small in molecular weight to allow sequencing by MALDI-TOF/TOF. The order of the fragments can be known by inserting the cyclic redundancy check (CRC), which is a check value to check whether there is an error in transmitted data, at the end of the information. We will synthesize a polymer with 512 repeating units for the first time and show the potential for storing digital information.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Control of Electronic Conduction Pathway in a Conductive MOF/Polymer Composite Film

Tae Gyun Hong, Dong Ki Yoon[1,*]

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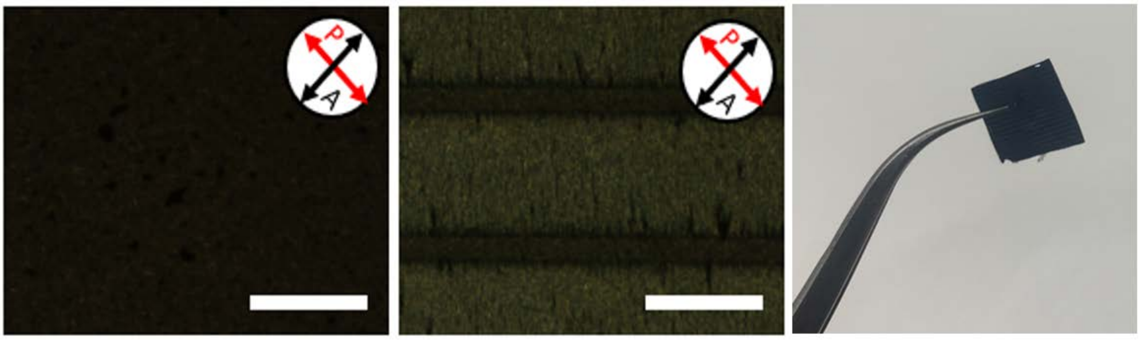
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

The vast majority of metal-organic frameworks (MOFs) are insulators, however because conductive MOFs have crystalline and porosity as well as electrical conductivity, they are gaining interest as a novel kind of hybrid inorganic/organic conductor. However, it is challenging to precisely evaluate the electrical transport of conductive MOFs due to their linked nanocrystal architecture. Currently, a widely used conductivity measurement method is a method of measuring conductivity in a bulk state by manufacturing MOF pellets, which is difficult to reflect intrinsic conductivity. So we aligned in electric field using the anisotropic crystal structure that most conductive MOFs have and then measured the intrinsic conductivity. Fine orientation control of MOF crystals is critical for performance optimization and device applications. Here, we synthesized a filled conductive polymer using conductive MOF in which electronic conduction path is controlled. Conductive MOF/Polymer Composite can be formed in a film form, and the conductivity varies greatly depending on the arrangement direction of MOF through an electric field.



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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

RAFT-Mediated Synthesis of Chelating Double-Hydrophilic Block-Copolymers for Zwitterionic Polysulfobetaine-Grafted Nanoassembly

Jiwoo Park, Sang-Min Lee[*]

Department of Chemistry, The Catholic University of Korea, Korea

Poly(sulfobetaine methacrylate) (pSBMA) has been studied as a representative zwitterionic polymers in aqueous solution. However, despite the high hydrophilicity and antifouling effect of SBMA, research has been limited due to the molecular weight-dependent solubility change by upper critical solution temperature (UCST). The goal of this study is to present a facile synthetic approach for poly(SBMA)-b-poly(methacrylate) block-copolymer by reversible addition and fragmentation chain transfer (RAFT) polymerization. The obtained copolymers can form core/shell-type self-assembled nanostructures by versatile metal chelation to the methacrylate blocks. The resulting metal-chelated nanostructures will exhibit great potentials for nanocatalysis and functional metal delivery in aqueous solution.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Metal-Chelating Block-Copolymers for Self-Assembled Nanocatalysts of Multi-Agent Loading Capability

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 can be prepared in a facile manner, which can then be employed as a delivery system for the biocatalytic agents.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

RAFT-Mediated Synthesis of Zwitterionic Block-Copolymers with Chelating Building Blocks for Coordination-Driven Self-Assembly

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(MA), block-copolymers through reversible addition and fragmentation chain transfer (RAFT) polymerization. The resulting copolymers can form a core/shell-type self-assembled nanostructure by versatile transition metal chelation in aqueous solution. Using the self-assembly strategy of chelating block-copolymers with multiple metal components, combinational nanostructures encapsulating versatile metallic cations can be obtained in a facile manner for enhanced functionalities.

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

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Randomly Glycated, Metal-Chelated Polysaccharides for Single-Chain Nanoparticle Formation

Yeonjoo Jung, Sang-Min Lee*

Department of Chemistry, The Catholic University of Korea, Korea

Chitosan as a biocompatible natural polysaccharide has been investigated as versatile polymeric scaffolds for the systemic delivery platforms and locally injectable gels. However, many of such chitosan derivatives often suffer from the low aqueous solubility over a wide range of pH conditions and extremely high viscosity, which significantly limits their broad applicability. Herein, the native chitosan has been non-enzymatically ligated with monosaccharides for the enhanced solubility at neutral pH, followed by the chemical modification with chelating agents that can be utilized as a multidentate ligand for versatile metal cations. The resulting metal-chelated, glycated chitosan has been self-aggregated into nanoscale structures. These structures will be able to exhibit the reversible cargo release by external stimuli such as pH changes. Their characterization and colloidal properties will be discussed.

Poster Presentation : **POLY.P-29**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

All-Polymer Solar Cells using a Dithienobenzothiadiazole-Based Polymer Donor with Siloxane Terminal Groups

Sung-Ho Jin[*], Yeong Soon Gal[1,*], Priyanka Yadav[2], Durgagayathri Rajalapati[2,*]

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Dithienobenzothiadiazole (DTBT) and benzodithiophene (BDT)-based wide band gap (WBG) polymer donors were investigated for use in All-PSCs. To further enhance the solubility, blend miscibility, and film morphology, a side chain made of siloxane was added to the BDT unit. Sil-1, a novel polymer, was created and thoroughly characterized. Sil-1 displayed a film absorption peak at 450 nm and an optical band gap of 2.19 eV. Between Sil-1, PM6 polymer donors, and PY-IT acceptor, complementary absorption and energy offsets were seen. The power conversion efficiency (PCE) of the PM6: Sil-1: PY-IT based All-PSCs was 14.7%, with an open-circuit voltage of 0.94 V, a short-circuit current density of 23.75 mA cm2, and a fill factor of 66.0%. The findings highlight Sil-1's potential as a potent donor, which is advantageous in the development of straightforward WBG polymer donors for effective All-PSCs.

Poster Presentation : **POLY.P-30**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Dopant-Free Terpolymeric Hole Transport Layer for Stable and Efficient Perovskite Solar Cells.

Chetan Lakshman, Sung-Ho Jin[1,*], Yeong Soon Gal[2,*], Jeonghyeon Park[3,*], Al-amin Md[3,*]

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[2]*Department of Fire Safety, Kyungil University, Korea*
[3]*Department of chemical materials, Pusan National University, Korea*

The efficiency of perovskite solar cells (PSCs) has recently improved, demanding a variety of capabilities for the charge-transport layers of the future. We adopted a random ternary copolymerization strategy for designing two terpolymers namely, P-0.8-E and P-0.8-T comprising benzothiadiazole (BT)-benzo[1,2-b:4,5-b´]dithiophene (BDT)-diketopyrrolo[3,4-c]pyrrole (DPP) backbone. The DPP core maintains the rigidity and planarity of the terpolymer structure. The merits of the narrow band gap P-0.8-E terpolymer include high hole mobility and better film formability. Accordingly, the suitable electronic properties of P-0.8-E revealed that it can act as a dopant-free hole transporting material (HTM) in PSCs. Remarkably, P-0.8-E exhibits a higher power conversion efficiency (PCE) of 20.5% over P-0.8-T (PCE of 18.3%) and CTRL (PCE of 14.6%), in dopant-free PSCs. Also, the P-0.8-E established good device storage stability (85 % of their initial PCEs for 1200 and 500 h).

Poster Presentation : **POLY.P-31**
Polymer Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Achieving High-Efficiency in Perovskite Solar Cells using Dopant-Free Polymeric Hole Transport Material

Zhiqing Xie, Sung-Ho Jin[1,*], Yeong Soon Gal[2,*], Donghyun Song[3,*], Jieun Lee[3,*]

Department of Chemical Materials The Graduate School Pusan National University, Pusan National University, China
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[3]*Department of chemical materials, Pusan National University, Korea*

Currently, Spiro-OMeTAD is still the most widely used hole transport material (HTM) in perovskite solar cells (PSCs).[1-2] However, pristine Spiro-OMeTAD shows low hole mobility and conductivity, which needs dopants, such as Li-TFSI and tBP, to improve charge transport performance. [3-4] However, the dopants are hygroscopic and accelerate the decomposition of the perovskite leading to poor device stability. Therefore, the exploration of doped-free, high-efficiency HTM material has always been the direction of our efforts. Here, a new polymer electron-donor material, Nap-SiBTz3, is designed and synthesized as a dopant-free HTM. A champion power conversion efficiency of 21.02% was achieved, which was higher than that of dope-free Spiro-OMeTAD (12.42%). Besides, Nap-SiBTz3 showed high hydrophobic property (water contact angle ≈ 101°), which is beneficial to the device’s long-term stability. These studies give useful guidance on exploiting efficient polymers as dopant-free HTMs in PSCs.

Poster Presentation : **POLY.P-32**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Defect-Curing of Uniaxially Aligned Poly(3-hexylthiophene) by Molecular p-Doping

Hokyeong Jeong

Department of chemistry, Hanyang University, Korea

Charge-transfer doping is a convenient method to enhance the electrical conductivity of the semiconducting polymer. In the case of the conjugated thiophene-based polymer poly(3-hexylthiophene) (P3HT), a 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) is known as the best candidate for P3HT charge transfer doping. In our previous report, our group developed the eutectic frictional transfer (EFT) method and fabricated P3HT thin film with high crystallinity. In this study, we combined charge-transfer doping with this $P3HT_{EFT}$ film using sequential doping. Strong anisotropic characteristics were analyzed by polarized UV, FT-IR, and Raman spectroscopy. Surprisingly, molecular p-doping not only maintains the backbone planarity but rather enhances it by minimizing the torsional reorganization barrier. The doped $P3HT_{EFT}$ film also showed high electrical conductivity of a maximum of 25 S/cm.

Poster Presentation : **POLY.P-33**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Paintable DNA Physical Unclonable Functions

Soon Mo Park, Dong Ki Yoon[1,*]

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

The debate concerning the legitimacy of the artwork continues despite several copyright protection mechanisms. The artists make every attempt to avoid these blunders by obtaining a certificate of authenticity or keeping their work prior to the second public exchange. However, the identification is open to falsification because of a lack of information security competence.Signatures or physical tags with identification numbers that serve as identifiers for the encryption key are frequent shields for artworks. Art dealers and auction houses utilize graphical and spectral labels such as radio-frequency identification tags (RFID), graphical barcodes, and watermarks. However, the primitives are not appropriate as security tags because cryptographic keys are deployed through a predictable process using symmetric protection and authentication approaches.In this paper, we offer brushstrokes, an artist-friendly platform for producing anticounterfeiting labels based on physical unclonable function (PUF). Deoxyribonucleic acid (DNA), which is naturally occurring, biocompatible, and environmentally acceptable, can be used for painting that demonstrates the entropy-driven buckling instability of the liquid crystal (LC) phase. The performance and dependability of line-shaped defect structures with intrinsic randomization as a source of PUF in the dried DNA film are extensively explored.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Preparation of a moldable cross-linked PMMA via direct amidation in the melt phase

Junsik Nam, Ji-Woong Park[1,*]

School of Material Science and Engineering, Gwangju Institute of Science and Technology, Korea
[1]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

Cross-linking of PMMA chains is an efficient strategy to improve mechanical and chemical strength. PMMA chains are interconnected by copolymerizing a cross-linker with the PMMA chain or substituting ester groups in PMMA with cross-linkers. However, the introduction of links between polymer chains reduces the processability of the polymer. For example, cross-linking of linear polymers forms insoluble solids that cannot be processed into a desired shape. Here, we show that a cross-linked PMMA can be simultaneously formed and molded in the molten state. PMMA beads and amine-functionalized cross-linker are simply mixed. Stepwise heating of the PMMA/cross-linker mixture makes it a melt phase. Simultaneously, amide linkages are formed between the cross-linker and PMMA chains to make cross-links. The resulting molded cross-linked PMMA has increased mechanical strength than the original PMMA while maintaining the optical properties of the original PMMA.

Poster Presentation : **POLY.P-35**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Self-Assembly of Discrete Bottlebrush Copolymers carrying Alternating Hydrophilic-Hydrophobic Pendants

Subin Park, Kyoung Taek Kim[1,*]

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

Amphiphilic copolymers are copolymers in which the hydrophilic monomers and hydrophobic monomers copolymerize in a regular specific sequence. The self-assembly behavior and structure of these polymers can be controlled by changing the monomer sequence distribution and the balance of hydrophilic and hydrophobic chains. Amphiphilic block copolymers induce intermolecular self-assembly to form multichain micelles, however, amphiphilic copolymers with hydrophilic and hydrophobic alternating sequences tend to fold during self-assembly to form unimer or multichain micelles. Herein, we report the synthesis of amphiphilic copolymers composed of the hydrophilic poly(ethylene glycol) (PEG) and hydrophobic alkyl groups alternatively attached to poly(malic acid) using iterative convergent method. The self-assembly of resulting amphiphilic copolymers can be analyzed by GPC comparing their structures in water or organic solvents. It is expected that the self-assembly behavior of alternating copolymers can be precisely controlled by the monomer sequence distribution.

Poster Presentation : **POLY.P-36**

Polymer Chemistry

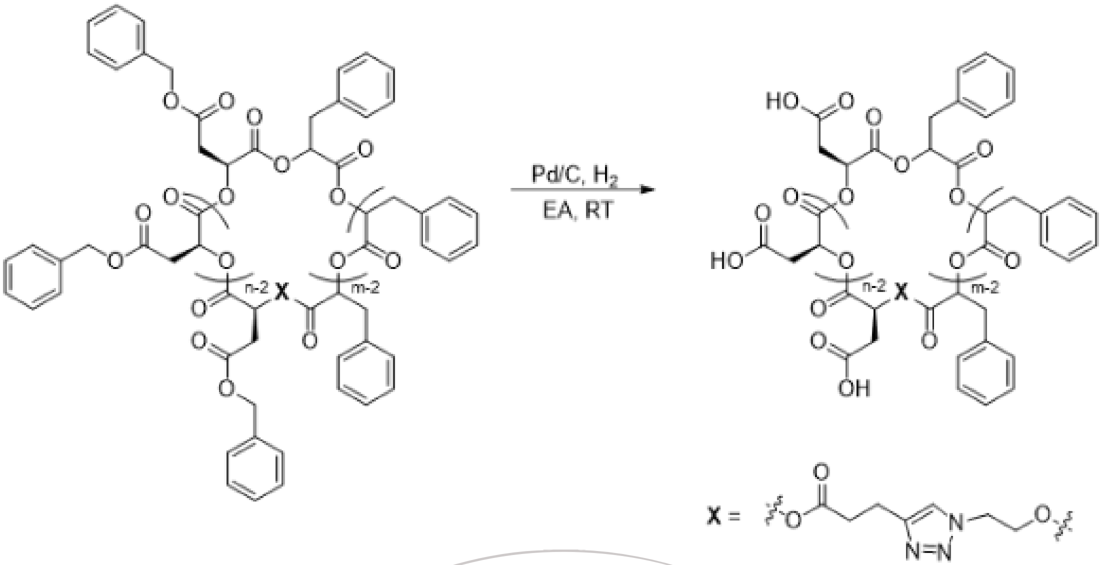
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Self-assembly of cyclic block copolymers containing poly(malic acid) and poly(phenyllactic acid) with discrete molecular weights

Seul Woo Lee, Subin Park, Kyoung Taek Kim*

Division of Chemistry, Seoul National University, Korea

Cyclic polymers attract interest because of their unique chemical and physical properties arising from their topological constraints of their chain conformations and absence of chain ends. Here, we report the synthesis of discrete cyclic block copolymers. Phenyllactic acid and benzylated malic acid were used to synthesize discrete homopolymers and oligomers. The resulting discrete polymers were linked to form block copolymers, followed by functionalization of chain ends for the copper-catalyzed azide-alkyne cycloaddition and hydrogenation to make amphiphilic cyclic block copolymers. The resulting linear and cyclic block copolymers were purified by using preparative size-exclusion chromatography and analyzed by GPC, NMR, and MALDI-TOF. We describe the effect of molecular weight and topology of the polymer chains on the morphology of the self-assembled structures of these monodisperse block copolymers.


Pd/C, H$_2$
EA, RT
n-2
m-2
X
HO
OH
O
X =
N
N=N

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Poster Presentation : **POLY.P-37**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Polymeric fiber patterning based on topological defect array of reactive mesogen

Changjae Lee, Dong Ki Yoon*

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

Oriented polymer fiber plays a part of interesting functions such as sensing, thermal insulation and control of wetting properties. Controlling the fiber orientation can be a key of tuning the applicability. However, patterning of polymer fibers is challenging because it requires a complicated multi-scale process. Here, three-dimensional patterning of polymeric fiber is reported by applying a designed electric field to a reactive mesogen dissolved in a liquid crystalline solvent. The applied electric field is derived from the crossed electrode cell, and its configuration can be diversified, resulting in different mesogen patterning. Solvent removal after in-situ photopolymerization completes the precisely patterned polymer fibers. These patterns can be microscopically analyzed and predicted through simulation. Finally, it is confirmed that the fabricated fiber array can induce a hydrophobic surface, showing an enhanced contact angle of 138º.

Poster Presentation : **POLY.P-38**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Biobased Thermoplastic Elastomers Based on Triblock Copolymers through ROMP from Vanillin Derivatives

Haneul Kim, Byungjin Koo*

Department of Polymer Science and Engineering, Dankook University, Korea

Thermoplastic elastomers (TPEs) are ABA-type triblock copolymers consisting of hard blocks at both ends and a soft block at the center. Exemplary TPEs are poly(styrene-*b*-butadiene-*b*-styrene) (SBS) and poly(styrene-*b*-isoprene-*b*-styrene) (SIS). Monomers for these TPEs are generally obtained from petrochemicals, and due to the potential depletion of petroleum resources, the needs to develop sustainable materials have received tremendous attention. In this work, we report hard blocks and soft blocks of TPEs that can be prepared from sustainable monomers. Specifically, we used vanillin, an active component of vanilla. The vanillin was functionalized with a norbornene carboxylic acid through a DCC coupling reaction of vanillin. We first attempted ring-opening metathesis polymerization (ROMP) of this vanillin-norbornene, exhibiting a number-average molecular weight (Mn) of 49,000 g/mol, a PDI of 1.23, and a glass transition temperature of 95 ℃. Having confirmed the excellent control of the homo-polymerization of the vanillin-norbornene, we executed the formation of TPE-like triblock copolymers, consisting of vanillin-norbornene at both ends and *n*-butyl-norbornene (in which *n*-butanol is also biobased) at the center. The triblock copolymerization was successfully performed via a sequential monomer addition through one-pot synthesis, and a step-wise increase in molecular weight was confirmed by GPC. A Mn of 25,900 g/mol and a PDI of 1.48 were observed. Scaling up this reaction and characterization of their mechanical properties are underway.

Poster Presentation : **POLY.P-39**
Polymer Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Octopi-Inspired Adhesive Patches Based on PDMS Microscale Suction Cups

Tae Woo Koo, Joon Kim, Hyuntae Ju, Seung Goo Lee*

Department of Chemistry, University of Ulsan, Korea

Acrylic-based adhesive patch leaves damage and residue on the skin surface and reduces adhesion in underwater environments. To overcome these problems, many researchers have developed bio-inspired adhesive patches to mimetic gecko feet and mushroom-shaped tips. However, without leaving chemical contaminants on the surface, the development of adhesive patches that can be repeatedly attached in wet and dry environments is still necessary. In this study, we report highly adaptable, biocompatible, and repeatable adhesive patches in various environments with microstructure inspired by the infundibulum of octopi suction cup. An octopi suction cup-inspired patches are fabricated by a simple molding process and controlling the meniscus of poly(urethane acrylate)(PUA) precursors using capillarity force. We performed the adhesion of the octopi suction cup-inspired patches using force gauge and showed excellent adhesion in Dry (19.7Kpa) and Wet (28.8Kpa) environments.

Poster Presentation : **POLY.P-40**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Impact Strengths of PLA/PS-based Ionomer Blends

Dahye Kim, Joon-Seop Kim*

Department of Polymer Science and Engineering, Chosun University, Korea

In this study, the Izod impact strengths of PLA and PS-based ionomer blends were measured. PS-based ionomers used in this work were sulfonated polystyrene (PSSA) and poly(styrene-co-methacrylate) (PSMA), neutralized with Li cation. It was observed that the impact strength of pure PLA was 15 J/m on average. When 10 wt% of PSMA ionomer containing 19 mol% ionic groups was added to PLA, the impact strength dropped sharply to about 5 J/m. In addition, it was found that the impact strength hardly changed even if the ionomer content in the PLA ionomer blend was further increased. There are two reasons why the impact strengths of PLA/ionomer blends are so low: First, the impact strength of a pure ionomer is 7 J/m on average, which is very low compared to the impact strength of PLA, and second, these ionomers enter the PLA matrix in phase-separated form and degrade the physical properties of the PLA itself.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Lignin-Polynorbornene Copolymerization via Ring-Opening Metathesis Polymerization of Lignin-Norbornene: Graft-to and Graft-from Approaches

Sumin Lee, Byungjin Koo[*]

Department of Polymer Science and Engineering, Dankook University, Korea

Lignin is the second abundant phenolic polymer biomass, whereas it has limited solubility in various solvents, which could restrict its applicability. We herein report chemical modification of lignin to form lignin-polymer conjugates by ring-opening metathesis polymerization (ROMP). The first step is modifying lignin with norbornene. Specifically, lignin phenolic groups and norbornene-carboxylic acids were connected in a Steglich esterification condition using DCC and DMAP. Next, a homopolymer having a ruthenium complex at the end of the polymer chain was prepared by ROMPing norbornene acetate, to which lignin-norbornene (LN) was reacted, which is a graft-to approach. The graft-to lignin-polynorbornene was soluble in various organic solvents, implying potential applications for composite materials. In another method, we attempted a graft-from approach, in which lignin-norbornene was first reacted with a third-generation Grubbs catalyst, followed by polymerization with norbornene acetate. Insoluble aggregates were observed, indicative of potential crosslinking between multiple norbornene moieties present on lignin. We are currently optimizing and analyzing the reaction condition to form graft-from lignin-polynorbornene. This method can contribute to lignin upcycling and applications.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of uniform and sequence-defined polystyrene

DoGyun Kim, Kyoung Taek Kim*

Division of Chemistry, Seoul National University, Korea

In recent times, there has been a surge of interest in the preparation of uniform and sequence-defined polymers, which is one of the most significant challenges in the field of polymer science. To this end, a range of orthogonal and efficient organic reactions have been employed for constructing sequence-defined macromolecules, including polyesters, polypeptides, and polypeptoids. However, despite these efforts, research on the synthesis of uniform aliphatic polymers such as polyolefins and polystyrene remain insufficient. In this presentation, we present our research findings on the synthesis of uniform and sequence-defined polystyrene

Poster Presentation : **POLY.P-43**
Polymer Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Self-Assembly of Polymer Cubosomes.

Carlos Grandes, Kyoung Taek Kim[1,*]

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

Self-assembled structures of simple amphiphiles such as lipids provide the structural basis of life such as cell membranes and organelles. Analogous to the polymorphism exhibited by lipids in vitro, lipid assemblies show complex morphologies including bicontinuous cubic mesophases (three-dimensionally regular membrane structures) in nature. There are numerous complex biological membranes throughout nature, for instance, mitochondrial intracellular membranes in amoebas, thylakoids in plant chloroplasts, and prolamellar bodies in tree shrew retinal cells. Additionally, biomembranes undergo a transformation from simple bilayers to cubic phases under stress or hunger. A lipid cubic phase is composed of three-dimensional structures in which the bilayers form an infinite periodic minimal surface that minimizes free energy. Inspired by the biological examples, lipid cubic mesophases has extensively studied to utilize the periodic arrangement of membranes internalizing water channel networks. Block copolymers (BCPs) are macromolecular analogs of lipids, which self-assemble into micellar and vesicular structures in aqueous solution. Therefore, the possibility of realizing complex polymer membranes analogous to biological membranes has been expected to appear from the self-assembly of BCPs in solution.Polymer cubosome is a highly ordered periodic porous polymer nanostructure with large-pore networks composed of inverse cubic mesophases of block copolymer (BCP) bilayers. Due to its large surface area, it has a potential to be used in separation, catalysis, drug delivery and nanotemplating by the introduction of desired functional groups on its surface. The structural requirements for preferential self-assembly of block copolymers into polymer cubosomes requires the hydrophilic block to have a branched architecture. Herein, we describe the synthesis of branched-linear block copolymers having hydrophilic blocks composed of three poly(ethylene glycol)s with an alkyne end group. These block copolymers self-assemble in aqueous solution to provide well-defined polymer cubosomes with densely populated surface functional groups.


Functionalized
Block copolymers
Solution Self-assembly
Surface functionalized
Polymer Cubosome

Poster Presentation : **POLY.P-44**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Impact strengths of bio-based PLA and petroleum-based sulfonated PPhO ionomer blends

Ingyeong Ryu, Joon-Seop Kim*

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In this study, to improve the applicability of PLA, we prepared blends with PLA and PPhO having a high glass transition temperature and measured their impact strengths. To enhance the miscibility of PLA and PPhO, PPhO was sulfonated and then neutralized with a monovalent cation. It was found that the impact strength of PLA decreased strongly upon blending with the ionomer. It was thought that the above results were probably due to the following two factors. First, SPPhO ionomer is a highly brittle polymer. Second, ion-ion interactions of SPPhO ionomer induce the formation of ionic aggregates. This leads to phase separation of ionomer itself in PLA matrix, which greatly reduces the bulk property of PLA.

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

New Pyrazine based pi-conjugated polymers for high performance dopant free perovskite solar cells

Jeonghyeon Park, Sung-Ho Jin[1,*], Yeong Soon Gal[2,*]

Pusan National University, Korea
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[2]*Department of Fire Safety, Kyungil University, Korea*

The new Polymer is designed and synthesized for fabrication of perovskite solar cells (PSCs) application. Poly[2-(5-(4,8-bis(5-(6-((2-hexyldecyl)oxy)naphthalen-2-yl)thiophen-2-yl)-6-methylbenzo[1,2-b:4,5-b']dithiophen-2-yl)-4-(2-ethylhexyl)thiophen-2-yl)-5-(4-(2-ethylhexyl)-5-methylthiophen-2-yl)pyrazine (BDTTN-PTEH) used as dopant-free hole transport material (HTM). The thermal, photophysical and electrochemical properties of BDTTN -PTEH were systematically investigated. BDTTN -PTEH exhibited a band gap of 1.96 eV with highest occupied molecular orbital (HOMO) of -5.596 eV and Lowest unoccupied molecular orbital (LUMO) of -3.636 eV. The electron withdrawing nature of pyrazine results in better intermolecular interactions, affording high hole mobility and charge transfer properties. Thus, optimized BDTTN -PTEH based device showed the power conversion efficiency of 17.5 % with open-circuit voltage of 1.09 V, a short-circuit current density of 24.45 mA/cm2 and a fill factor of 64.89 %. This result indicated that pyrazine based polymer have great to further development of HTM.

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Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Beta Phase Enhancement of PVDF by Adding Thermally Decomposable Molecules, Made from In-situ Reverse Diels-Alder Reaction

Jinwoo Choi, Youngjong Kang[1,*]

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

An additive, 1,4-butadiene sulfone (BDS), which generates H2SO3 by in situ thermal retro-Diels-Alder decompositions, is used for preparing high β-phase PVDF films. Because of preferential multiple non-covalent interactions of sulfurous acid with all-trans configuration of PVDF, β-phase PVDF is spontaneously induced without mechanical drawing and/or extensive thermal annealing process. PVDF films cast from PVDF/BDS/water solutions exhibit high β-phase content (fβ = 95%) when the BDS concentration is only cBDS = 1.0 wt%, which is confirmed by POM, SEM, FT-IR, DSC, and 2D GIWAXS. Because of high β-phase content, PVDF films prepared by using BDS exhibit excellent ferroelectric and piezoelectric properties (Ec = 50 MV/m, Pr = 5 μC/cm2 and d33 = ~–25 pm/V). Furthermore, a triboelectric nanogenerator (TENG) developed with high β-phase PVDF film exhibits enhanced performance as 2.5 times higher than neat PVDF film in output charge density, allowing reliable operation of conventional electronic devices.

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Poster Presentation : **POLY.P-47**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Conductive Block Copolymer composed of Amorphous and Crystalline Blocks via Glassy Macroinitiator.

JunWoo Kang, Kyoung Taek Kim[1,*]

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

Thiophene is used in various fields as a monomer of conducting polymer. However, as the crystallinity of polythiophene changes depending on the functional group of thiophene, the thermoelectric properties such as electrical conductivity change, so polythiophene with high electrical conductivity has a problem that it has low solubility and is fragile and difficult to handle. Physical properties can be controlled by block copolymerization with an amorphous block such as PDMS, but some thiophenes such as EDOT have too low solubility and are difficult to synthesize. To solve this problem, we synthesized PDMS having an initiation site of thiophene polymerization and proceeded with polymerization. As a result, it was confirmed that a blockcopolymer of PDMS and thiophene was synthesized. Our research will contribute to the synthesis of conducting polymers in more diverse ways.

Poster Presentation : **POLY.P-48**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Correlation lengths determination of star-poly(ethylene oxide) networks by using small-angle scattering measurements

Jungju Ryu[*], **Daewon Sohn**[1,*]

Department of Chemistry and Research Institute for Convergence of Basic Science, Hanyang University, Korea

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

Poly(ethylene oxide) networks were investigated in terms of the types of links of functional end groups that can have trigonal and linear connections. Regarding the linear crosslinking, X-ray scattering measurements observed homogeneous structures, and rheological property tests showed relatively strong properties. We also explore the nano-structures established with linear linkages by using contrast-variation neutron scattering techniques. The results revealed that the end groups supported the correlation lengths corresponding to the polymer size and the shadow spaces associated with the linkages between end groups. This study provides the fundamental ideas that can assemble the networks.

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Particle diffusion detection by using evanescent wave light-scattering

Jungju Ryu[*], **Daewon Sohn**[1,*]

Department of Chemistry and Research Institute for Convergence of Basic Science, Hanyang University, Korea

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

We designed the evanescent wave light scattering that can detect particle diffusion near the wall. The instrument was established to explore the particles that can interact with silica-based surfaces. The penetration depth was controlled depending on laser wavelengths and incident angles. Here, we demonstrate how we can get the scattering signals of latex particles in the range of several nanometers between the aqueous media and the silica-based wall. The results showed that the diffusive characteristics near the wall slow down from that of the bulk system. This study suggests a method to observe the interaction of the particles at the interfaces.

Poster Presentation : **POLY.P-50**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Highly soluble copper(II) phthalocyanine-based organic photodetectors with fast signal response

Doyeong Yeo, In Hwan Jung[1,*]

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[1]*Department of Organic and Nano Engineering, Hanyang University, Korea*

Phthalocyanine (Pc) based organic dyes composed of macrocyclic rings have been grown attention as an alternative material of conjugated polymers for use in organic photodetectors (OPDs) due to their promising properties such as high chemical and thermal stability, redox properties, and high absorption coefficient value in UV-VIS wavelength region. However, the poor solubility of Pcs makes a limitation of their usage as an application for optoelectronics. In order to overcome this issue, we synthesized a novel Pc-based organic dyes for the active materials of OPDs. The synthesized dye exhibited not only a good solubility in organic solvent but also strong Q-band absorption in the visible area. The bulk heterojunction OPDs was prepared by blending it with PC71BM, and the fabricated devices exhibited the specific detectivity (D*) value of 3.04 × 1011 and 1.07 × 1011 Jones and under about 0.1 mW/cm2 of 532nm and 680 nm light illumination, respectively. In addition, CuPc-HT based OPD exhibited an extremely high -3 dB cut-off frequency of about 0.1 MHz and an ultrafast signal response time of approximately 9 μs under modulated 532 nm LASER illumination at -1.0 V bias.

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Acoustic focusing method for single micro-sized particles

<u>Hoyeon Lee</u>, Daewon Sohn[1,*]

Graduate student in chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Flowcytometry holds the key to the future of diagnostics. With antibody-antigen fluorescence dyes, we can discover many information about cells at once. One of the tools that can effectively center the particles is acoustic focusing, which allows us to detect dye molecules more precisely and increase resolution. Piezoelectric material microchannels with a rectangular 100μm size were used in this experiment. The 7.39MHz wave is used to create constructive interference. In here, 4um particles can be centered at up to 80μL/min flow rates. Additionally, particles of 1.33um size can also be centered at flow rates of 10μL/min. According to this study, there is a possibility of direct detection of bacteria.

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Poster Presentation : **POLY.P-52**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Modification of alkyl group with aryl group side chain in small molecule non-fullerene acceptor for organic solar cells

Chanbeom Park, Eunhee Lim*

Department of Applied Chemistry, University of Seoul, Korea

To further advance organic solar cells, various molecular synthetic strategies have been proposed and applied in designing donor and acceptor with desirable physical properties. Among the building blocks of various molecular structures, there is no alkyl group with an aryl structure in the side chain, or research on length control and bulkiness is sluggish. The effect of the cyclic alkyl group having an aryl structure on molecular aggregation depends on the position of substitution and the type of molecular structure. The introduction of an alkyl group having an aryl structure may control intermolecular aggregation. This study, non-fullerene acceptors (NFA) were easily synthesized by changing alkyl with aryl group chains to terminal structures within a simple molecular structure. It can provide a useful side-chain for the design of NFAs.

Poster Presentation : **POLY.P-53**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Effect of alkyl side chains on physical properties and device performance of Non-fused Non-fullerene acceptors in organic solar cells

Guseon Kim, Eunhee Lim[*]

Department of Applied Chemistry, University of Seoul, Korea

Organic solar cells (OSCs) have emerged as future energy generators and made great efforts to improve OSCs performance. Non-fullerene acceptors (NFAs) can be easily synthesized in high yields and their energy levels, UV-vis absorption, and the film morphology can be adjusted. In these organic solar cells, physical properties can be changed through various molecular structural modifications. Among them, we study on alkyl-side-chain-engineering. We report the synthesis and characterization of the bulky-alkyl side chains. In this study, we investigated how these bulky side chains influence solubility, self-assembly, charge mobility, molecular packing and the structure property relationship of the acceptors.

Poster Presentation : **POLY.P-54**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Asymmetric core non-fullerene small molecule acceptor for high performance organic solar cells

Dayoung Kim, Guseon Kim, Eunhee Lim*

Department of Applied Chemistry, University of Seoul, Korea

Organic solar cells (OSCs) are attracting great attention due to their advantages of translucency and flexibility. In order to increase the power conversion efficiency (PCE) of OSCs, studies on asymmetric non-fullerene acceptors (NFAs) are being actively conducted. Recently, studies have been reported that the well-known alkyl side chain of Y6 is modified to have asymmetry so that molecular packing can be well controlled. In this work non-fused asymmetric NFA, based on a benzothiadiazole-thiophene-containing asymmetric core has been developed. Synthesized NFA absorb the wide UV-vis area from 350 to 700 nm by SVA treatment, due to the unique aggregation which has either J- and H- aggregation and exhibit sufficient solubility and thermal stability for fabricating devices. This study provides a novel strategy to construct asymmetric NFA for efficient organic solar cells.

Poster Presentation : **POLY.P-55**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

High-brightness photoluminescent dispersion paint with self-flame retardant function and visibility even in the haze caused by fire.

Jeil Kim

song-hyun L&C, Korea

1. Background and necessity of the study - Safety problems due to lack of night activities and lighting facilities - Increasing demand for the development of materials that can emit light without a separate energy source2. Necessity of technology development - The current flame retardant material is a brominated flame retardant with excellent effect, but dioxin is generated during combustion - It is necessary to develop a flame retardant that not only has excellent flame retardancy, but also has low harm, low flammability, and low corrosion properties.3. Research Objectives - Development of high-brightness luminescent paint with flame retardant performance that can withstand high temperatures - Photoluminescent fluorescent paint with composite phosphorus flame retardant function: Safe evacuation in case of emergency with photoluminescence/flame retardant function 4. Research Methods - Development of nitrogen/phosphate flame retardant manufacturing technology without added halogen elements - Development of photoluminescent coatings with improved brightness performance that overcome the shortcomings of existing coatings with weak visibility5. Research results - Development of high-brightness photoluminescent dispersion applied to reactive flame retardant - Development of reactive type 2 handover or nitrogen/phosphate flame retardant material flame retardant to replace existing additive type flame retardant products Improve workability and quality6. conclusion - Using flame retardant photoluminescent paint applicable at high temperature (400°C), it is applied to various places such as emergency fatigue inside public institution buildings, emergency fatigue inside manufacturing plants and construction sites, emergency signs inside road tunnels, and emergency information signs.

Poster Presentation : **POLY.P-56**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Mechanical properties and morphology of poly(butyl acrylate) ionomers neutralized with various cation

Kwang-Hwan Ko, Joon-Seop Kim[1,*]

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The effects of the type of cation on mechanical properties and morphology of poly(butyl acrylate) ionomers were determined using DMA, SAXS techniques. As a result of the SAXS experiment, the q_{max} value at which the apex of the peak appeared in the SAXS peak of each sample shifted at a smaller angle as the size of the cation increased. In the case of iomers neutralized with monovalent cations, the degree of q_{max} value was in the order of Cs^+-ionomer > K^+-ionomer > Na^+-ionomer > Li^+-ionomer, and in the case of divalent cations, the order was Zn^{2+}-ionomer > Ba^{2+}-ionomer. This result seems to be because the larger the size of the cation radius, the larger the distance between the scattering centers, which is because the total number of multiplets decreases.

Poster Presentation : **POLY.P-57**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Recyclable polyurethane adhesives based on dynamic oxime-carbamate bond

Ji Won Jang, Changsik Song[1,*]

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

Polyurethane is used in many fields, among which cross-linked polyurethane has been preferred as an adhesive because of its excellent mechanical properties and high adhesion. However, there is a limitation that detachability and recycling are impossible, and recently, studies to overcome these disadvantages have been actively conducted. Among them, studies that introduce dynamic covalent chemistry are attracting attention. In this study, detachable and recyclable cross-linked polyurethane was synthesized by introducing an oxime-carbamate bond, one of the dynamic covalent bonds. To introduce the oxime-carbamate bond, dimethylglyoxime, which is commercially available and has an oxime-carbamate bond, was used as a chain extender. In addition, ethylene glycol, which has no reversible bond, was used as a chain extender to compare adhesive strength with polyurethane.

Poster Presentation : **POLY.P-58**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Quartz Crystal Microbalance Sensor For Chemical Warfare Agent Using Trisaryl Phosphoric Triamide Based Resin

Jaeyoung Heo, Changsik Song[1,*], Han yong Bae[1]

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

At the present time when chemical weapons are being used in warfare, we can be exposed to attacks using chemical substances at any time. Therefore, it is necessary to be aware of the attack using the Chemical Warfare Agent and continue research to enable detection in the actual field. We designed and synthesized a trisaryl phosphoric triamide-based resin receptor, a new material that can detect CWA by using a weak hydrogen bond with CWA gas and -OH functional group. After synthesizing Trisaryl Phosphoric Triamide-based materials, we proceeded with a simple reaction with Epoxy-based materials to form -OH functional groups. In addition, by introducing 1,6-Diaminohexane with a long alkyl group, the coating property of the prepared receptor was improved, and it was confirmed that the coating property of the material was improved compared to the conventional method. The synthesized receptor was coated on a QCM sensor by a simple drop-casting method, and CWA simulant 2-CEES was measured. As a result of the measurement, it was confirmed that the receptor showed good reactivity to the 2-CEES gas, and the reactivity also changed proportionally with the change in the concentration of the 2-CEES gas. From these results, it was confirmed that the prepared receptor was reactive to 2-CEES. In addition, it was confirmed that the detection ability of 2-CEES using our developed receptor can be detected at r.t., unlike previous studies that required high temperature.

Poster Presentation : **POLY.P-59**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Self-healable and photo-responsive adhesives from fully bio-based epoxy polymers

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

Fully bio-based epoxy polymers made from cinnamic acid offer several advantages over traditional petroleum-based adhesives. They are environmentally friendly, as they are made from renewable resources and have a lower carbon footprint. They are also less toxic, as they do not contain harmful chemicals such as bisphenol A (BPA) or other harmful additives commonly found in petroleum-based adhesives. So, we designed fully bio-based epoxy polymers made from cinnamic acid for developing photo-responsive and self-healable adhesives that are both strong and environmentally friendly.

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Poster Presentation : **POLY.P-60**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Living Anionic Polymerization of Styrene Derivative Containing Triphenylamine Moiety

Woo-jae Jang, Beom-Goo Kang[*]

Department of Chemical Engineering, Soongsil University, Korea

In this research, A new polymer poly(A), which has triphenylamine group as hole-transporting moiety, was synthesized by living anionic polymerization. The anionic polymerization of (A) was performed in THF at -30 ℃ for 10 min without additives. The well-defined poly(A)s with predictable molecular weight (20,000-120,000 g/mol) and narrow molecular weight distribution (1.08-1.12) were obtained quantitatively. The anionic reactivity of living (A) was confirmed by block copolymerization with styrene (S) and 2-vinylpyridine (2VP). Their thermal and optical properties were also investigated. And finally, poly(A) was used as hole-transporting material (HTM) in multilayer OLEDs devices. To make multilayer structure, cyclohexanone was used as an orthogonal solvent, in which emitting material (F8BT) can soluble but poly(A) is insoluble. The device performances showed that poly(A) can be a new HTM in OLEDs

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Poster Presentation : **POLY.P-61**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Semi-conductive micellar networks of all-conjugated diblock and triblock copolymer blends

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Division of Chemistry, Seoul National University, Korea

When block copolymers (BCPs) self-assemble into one-dimensional (1-D) nanostructures such as worm-like micelles in solution, the solvent-insoluble blocks of the polymers form the core of the micelle, which is surrounded by the solvent-soluble polymer blocks. In this spontaneous process, polymer nanowires are formed with a localized polymer domain, and their desired chemical and physical properties originate from the chemical structures of the core-forming polymer blocks. In particular, all-conjugated BCPs composed of amorphous and crystalline polymer blocks could be unique building blocks for creating 1-D nanowires in solution by crystallization-driven self-assembly (CDSA). Here, we report the preparation of organogels by the CDSA of a blend of diblock and triblock copolymers composed of crystalline poly(3-hexylthiophene) (P3HT) and amorphous poly(3-ethylhexylthiophene) (P3EHT), which comprise conjugated polymer blocks. The living CDSA of the blends of P3HT-b-P3EHT and P3HT-b-P3EHT-b-P3HT in anisole leads to the cross-linking of the 1-D nanowires of P3HT-b-P3EHT; this is achieved via the intercalation of the P3HT blocks of the triblock BCPs into the nanowire cores. The resulting gels of the semi-conductive nanowires rendered flexible and porous films upon drying, which showed conductivity (~80 S/cm) upon doping with AuCl3.

Poster Presentation : **POLY.P-62**

Polymer Chemistry

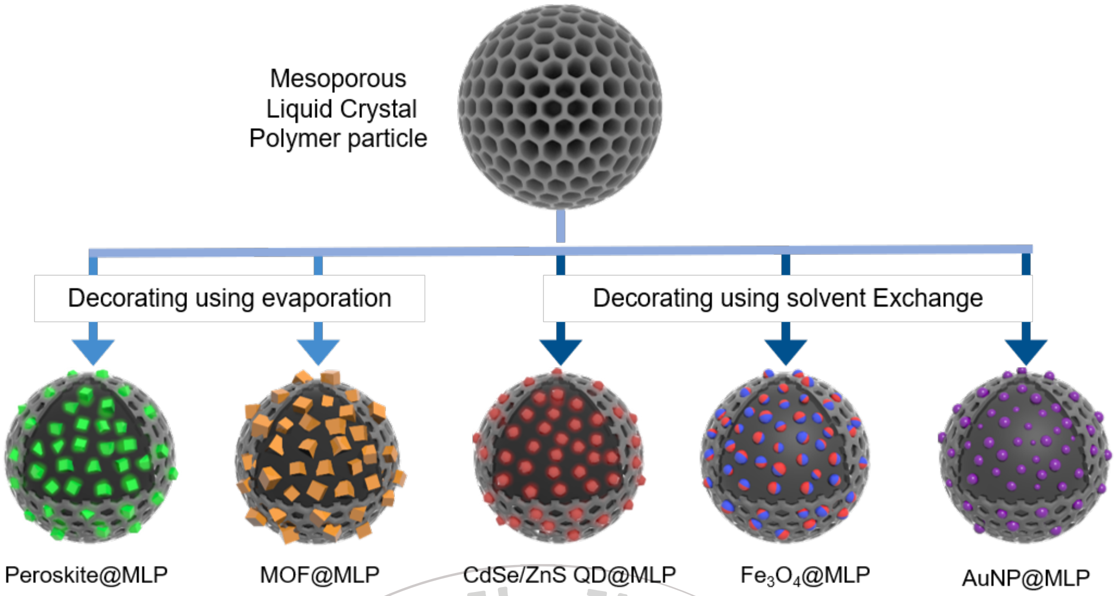
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Universal Incorporation Nano Material in Mesoporous Liquid Crystal Polymer Particles

Geonhyeong Park, Dong Ki Yoon*

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

The development of functional polymers that can respond to external stimuli has opened new possibilities for various fields, including biomedical engineering, energy, electronics, and environmental technologies. The integration of inorganic materials with superior properties into the polymer matrix is a commonly employed strategy to fabricate functional polymers, resulting in unique properties that cannot be achieved solely by the polymer constituents. Liquid crystal (LC) polymers are a promising candidate as a matrix material for organic-inorganic composite polymer due to their low density, high thermal and solvent stability, and the ability to be formed into diverse shapes. In this study, we propose a universal strategy for incorporating inorganic nanoparticles into mesoporous liquid crystal polymer particles (MLPs). The MLPs were synthesized using reactive mesogen and non-reactive mesogen via emulsion polymerization, resulting in the formation of highly cross-linked mesoporous polymer particles. Two strategies were employed for the incorporation of functional inorganic nanoparticles into MLPs, including synthesizing nanoparticles within MLPs through solvent evaporation and incorporating pre-synthesized nanoparticles into MLPs via solvent exchange. These integrations impart properties such as fluorescence, photo-catalytic behavior, magnetism, and photothermal effects that are not expressed by MLP alone, and MLPs can provide protection to delicate nanoparticles from damage or decomposition. This work highlights the potential of using LC polymers as a matrix material for organic-inorganic composite with applications in diverse fields, such as biomedical engineering, electronics, energy, and environmental technologies.


Mesoporous
Liquid Crystal
Polymer particle
Decorating using evaporation
Decorating using solvent Exchange
Peroskite@MLP
MOF@MLP
CdSe/ZnS QD@MLP
Fe_3O_4@MLP
AuNP@MLP

Poster Presentation : **POLY.P-63**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Preparation of Adhesive, Self-healing, and Biocompatible Hydrogels based on Schiff base Linkages

Hend Hegazy, Changsik Song[1,*]

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

Tissue adhesives play a crucial role in treating injuries and promoting wound healing and tissue sealing. While cyanoacrylate and fibrin glue are the most commonly available commercial adhesives, they have limitations such as being toxic to cells and not having strong adhesive properties, which restricts their use in biological applications. As a result, developing an adhesive system that can enhance tissue repair and closure while being non-toxic is a crucial yet challenging task. In this study, to address the drawbacks of commercial adhesives, we created biocompatible hydrogels through the crosslinking of amino-functionalized polyaspartamide and dextran aldehyde, a naturally occurring substance, using Schiff base chemistry. We then evaluated the adhesive properties of these hydrogels. The degree of crosslinking can be influenced by the proportion of amine and aldehyde functional groups in the polymers, as well as the concentration of the polymers. We evaluated the adhesive characteristics of the hydrogels using rheometer and lap shear tests. The polyaspartamide-based adhesive hydrogels displayed high mechanical strength and self-healing abilities, as well as superior adhesive properties compared to fibrin glue, indicating their potential for use in tissue adhesion applications

Poster Presentation : **POLY.P-64**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Micro-Sized Triangular Structures by Stacking of Stereocomplexes of Discrete Poly(lactic acid)s

Jae Hak Lee, Kyoung Taek Kim[1,*]

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

Discrete polymers herein, which are composed of two oligo(lactic acid) domains, [DLAn] and [LLAm] (n>m), by using an exact number of D- and L-latic acids, respectively. Interestingly, stereoblock copolymer having a mismatch in lactic acid unit formed micro-sized triangular structures. This is probably due to the stacking of stereocoplexes which is induced by extra D-lactic acids constituting mismatched stereoblock copolymers. The effect of the extra D-lactic acid units in mismatched stereoblock copolymers were investigated by decreasing the extra units. Depending on the degree of extra units. size and thickness of assembled structures were changed. We believe that these results will help prepare materials of various sizes.

Poster Presentation : **POLY.P-65**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Improvement of Properties of Perfluorinated Ionomer Blend Film

Jina Heo, Young-Je Kwark*

Department of materials science and engineering, Soongsil University, Korea

This study focuses on the development of ion exchange membranes using ionomers, which are random copolymers with sulfonic acid groups that form ion channels via a phase-separated structure consisting of a hydrophobic backbone and a hydrophilic side chain. The resulting polymer electrolyte membranes (PEMFC) are critical components in fuel cells, requiring high ion conductivity characteristics, typically expressed as equivalent weight (EW).To improve ion conductivity, blends of ionomers with different EW values were attempted. Ionomers with different EW were synthesized by controlling Perfluoro-2-(2-fluorosulfonylethoxy) Propyl Vinyl Ether (PSEPVE) and EW was calculated by using pH meter. Films were made by solution casting by mixing the ionomer with other EWs. Chemical durability was evaluated via the Fenton reaction, and surface properties of the film were analyzed through contact angle measurements. Through the analysis results, the claims of single film and blend film were cited.

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Poster Presentation : **POLY.P-66**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

The effect of stabilizer in miniemulsion polymerization of perfluorinated ionomers

Joon Young Koh, Jina Heo[*], Young-Je Kwark[1,*]

Material science and engineering, Soongsil University, Korea
[1]*Soongsil University, Korea*

Perfluorinated ionomers have shown great promise as proton exchange membranes (PEMs) in fuel cell technology. These ionomers, which are composed of tetrafluoroethylene and perfluorovinyl ether with sulfonic acid functional groups, are synthesized using miniemulsion polymerization. However, in order to prevent Ostwald ripening, a good stabilizer (cosurfactant) is required, which should have high insolubility in water and be soluble in the monomer. Additionally, the stability of the miniemulsion may be influenced by the molecular weight and chain length of the stabilizer.In this study, we attempted copolymerization of ethanesulfonyl fluoride and tetrafluoroethylene (TFE) using various stabilizers, including perfluoropolyether (PFPE), perfluorocyclic ether, perfluorosulfonylfluoride ethyl propyl vinyl ether, and perfluorotripentylamine. The effects of each stabilizer on the equivalent weight (EW) and melt flow index (MFI) of the ionomer, as well as the stability of the monomer droplets, were investigated. These findings have implications for the development of improved stabilizers and miniemulsion polymerization techniques for the synthesis of perfluorinated ionomers.

Poster Presentation : **POLY.P-67**

Polymer Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Characterization of Fluorosilicone Resins with Various Contents of a Vinyl Group

Hansan Ko, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Recently, as the demand for improving the physical properties of fluorinated rubber has increased, research on fluorinated silicone resin has been actively conducted. If the vinyl group content is high based on the same molecular weight as fluorine silicone resin, it is expected to have a positive effect on strengthening the rubber properties. Therefore, we synthesized fluorinated silicone resins by controlling the contents of a vinyl group and compared their properties. As a result, the synthesized resin was analyzed by Si-, H-NMR, GPC, and TGA, and the molecular weight of the synthesized resin was about 1100 ~ 1500 based on Mw. It was confirmed through H-NMR that a vinyl group was introduced and through TGA analysis that the rest of the monomers were removed.

Poster Presentation : **IND.P-68**

Industrial Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Non-Destructive Evaluation of a Metakaolin Geopolymer Solidification Utilizing 3-Dimensional X-ray Computed Tomography

Hyung-Ju Kim

Korea Atomic Energy Research Institute, Korea

Geopolymers display lots of potential as suitable solidification agent candidates for 14C immobilization. However, internal structure characterization remains as unknown territory without destruction of the geopolymer for conventional characterization techniques such as electronic microscopy; an incomplete solution for investigating solidifications. X-ray Computed Tomography (XCT) enables non-destructive evaluation of solidification in terms of both internally and externally without any destruction. Metakaolin was activated by either sodium hydroxide (NaOH) or potassium hydroxide (KOH) to form a geopolymer solidification. In the case of using NaOH as the activator, XCT analysis indicates a heterogenous geopolymer matrix, suggesting incomplete polymerization, and internal cracking. In contrast, samples using KOH as an activator show a homogeneous geopolymer matrix, suggesting complete polymerization void of internal cracking.

Poster Presentation : **IND.P-69**
Industrial Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Solid-state NMR probes: Design and manufacture for analysis of various materials

Minseon Kim, Yongae Kim*

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Solid-state NMR has the advantage of being able to measure almost all ranges of samples, such as amorphous powder as well as oriented crystalline samples like polymer fibers, cell membrane proteins, and liquid crystals. Selecting a probe suitable for the purpose according to various materials is also a very important step in obtaining desired results in solid-state NMR. In this study, we will discuss how to design and fabricate efficient and durable probes for various materials. A home-built 400 MHz narrow-bore (NB) and wide bore (WB) ^{1}H-^{15}N solid-state NMR probe and a home-built 800 MHz NB ^{1}H-^{15}N solid-state NMR probe for lossy samples, 400 MHz and 500 MHz NB ^{19}F-^{13}C solid-state NMR probe for analyzing nanomaterial and 600 MHz NB ^{19}F-^{7}Li solid-state NMR probe with solenoid coils for investigating Li-ion battery were fabricated in our lab. In addition, in order to study the structure of a biological sample, an environment mimic to the natural state of the sample, such as a lipid bilayer, should be provided. Since the molecular motion of the lipid bilayer is slow, a solid-state NMR probe of an oriented bicelle sample is also proposed in this study. Preliminary NMR data was collected for all home-built probes to demonstrate their efficiency.

Poster Presentation : **IND.P-70**

Industrial Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Anti-PVY activity that is inversely proportional to the drug concentration

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Since potatoes are an important food resource worldwide, damage from PVY could adversely affect the global economy. Nevertheless, effective pesticides to combat PVY have not yet been developed. In the process of developing a new anti-PVY pesticide, we discovered a new drug candidate and developed a stereoselective synthesis method. Currently, various studies are being conducted for commercial use, but in the develop process, some difficulties are encountered in the face of phenomena different from common scientific knowledge. Generally, in the absence of toxicity, the concentration and activity of a drug are proportional to each other. However, the PVY inhibitory effect of the our candidate molecule was higher as the concentration was lower. In this presentation, we would like to hear the opinions of many experts and discuss such phenomena.

Poster Presentation : **IND.P-71**

Industrial Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Mass Spectrometry Imaging Analysis of OLED using LDI TOF-MS.

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Recently, in the display industry, mass spectrometry is also used to analyze the composition of the materials used to manufacture display industry. With the increasing popularity of OLED (Organic Light Emitting Diodes) displays, it is essential to understand the factors that contribute to their performance degradation over time, and mass spectrometry can provide valuable insights into the composition of the materials used to manufacture these displays. One of the critical factors in OLED degradation is the presence of impurities or contaminants in the OLED device, which can react with other materials and reduce performance. The LDI TOF-MS, equipped with a high-resolution microscope, is a powerful analytical method for analyzing impurities and contaminants directly from the OLED without laborious sample preparations. With its 5 μm spatial mass imaging resolution, this technique can detect contaminants or impurities of 10 μm or less that are commonly observed in defective panels. To facilitate OLED analysis, an OLED material database has been established. Both cation and anion information are used to obtain structural information, providing a comprehensive understanding of the composition of the OLED materials. This information can help identify impurities and contaminants that may be contributing to OLED degradation, allowing manufacturers to optimize their production processes and improve the performance and lifespan of OLED displays. Overall, mass spectrometry is an essential tool in the analysis of OLED materials, providing valuable insights into the factors that contribute to their performance degradation over time. Its use in the display industry is a promising development that will undoubtedly help drive the continued improvement of OLED technology.

Poster Presentation : **INOR.P-1**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Controlled Ring Opening Metathesis Polymerization of Norborne by Iminomethyl-hydroxyl Ligated Tungsten Complexes

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A series of tunsgten complexes ligated to iminomethyl-hydroxyl derivatives, [L_nWCl_4] and [L_nWOCl_2] (L_n = L_A and L_B), where L_A is (Z)-1-(((2-hydroxyphenyl)imino)methyl)naphthalen-2-ol, and L_B is (Z)-5-chloro-2-(((2-hydroxyphenyl)imino)methyl)phenol, have been synthesized by the direct ligation of $WOCl_4$ or/and WCl_6 with ligands, leading to the displacement of two chloride units from the metal center. The synthesized complexes's structures have been verified by spectro-analytical techniques. Activated with triisobutylaluminium (TIBA) as promotor, the synthesized complexes have been demonstrated to form a highly active catalytic system for Ring Opening Metathesis Polymerization (ROMP) of cyclic olefins such as norbornene (NB). 100% conversion of NB into polyNB (PNB) has been observed by ^1H NMR with respect to the reference tetraline within 10 minutes.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Furan-Derived Schiff Base Complexes; Synthesis, Characterization, Anti-urease and leishmanicidal Properties, and Molecular Docking

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In this study, we planned to synthesize CH_1-symmetric furan-derived Schiff base complexes with zinc, copper, and cadmium metal centers with the hope that the use of these metal complexes would likely have great potential as anti-urease and anti-leishmanial agents. (E)-N^1,N^1-diethyl-N^2-(furan-2-ylmethylene)ethane-1,2-diamine (DEF), and the corresponding M(II) complexes, [DEF(M)X_2] (M = Cu, Zn; X = Cl; M = Cd, X = Br), were synthesized and structurally characterized. X-ray diffraction studies revealed that the geometry around the center of the M(II) complexes, [DEF(Zn)Cl_2] and [DEF(Cd)Br_2], could be best described as a distorted tetrahedral. Complexes were tested in vitro for their urease inhibitory potential against Jack bean urease and Bacillus pasteurii urease (BP urease). [DEF(Cd)Br_2] exhibited prominent inhibitory potential against JB urease (IC_{50} = 4.5±0.17 μM), and BP urease (IC_{50} = 5.0±0.13 μM) compared to the standard thiourea (IC_{50} =12±0.62 and 9.80±0.90 μM). Additionally, molecular docking confirms the probable binding modes of the active complexes into the crystal structure of JB urease. The studied complexes also exhibited superior leishmanicidal properties.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Robust Soccer Ball-like Self Assembly by Monolayer Array of Edge-Sharing 2D-SiO2 Nanosheets

Sunwoo Jang, Kyeong-bin Kang[1], In Su Lee[2,*]

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Despite several advantageous aspects of hollow microspheres, template-free synthesis of micro-sized assembled structures, especially from two-dimensional (2D) nanomaterials, remains challenging due to the strong Van der Waals (VdW) attraction between the faces of 2D nanoscale building units. Here, we reveal the unique soccer ball-like edge-to-edge oriented self-assembly of 2D-SiO2 nanosheets by engaging enough electrostatic face-to-face repulsion to overcome the VdW attraction. In detail, we overcame the strong VdW attraction between faces using electrostatic repulsive force through silica encapsulation, and induced edge attraction using the structural properties of 2D materials with significantly different curvature of edges and faces. More interestingly, we confirm that 2D-SiO2 nanosheets have different flexibility depending on silica thickness, which allows various self-assembly structure. In order to create robust soccer ball-like hollow microsphere enclosed by a monolayer array of edge-sharing 2D-SiO2 nanosheets without template, proper harmony of surface charge and flexibility is required. Additionally, hollow microsphere developed in this study shows superior structural robustness without any additional treatment and it is expecting to be applied to high performance catalyst for various organic chemical reactions. This creative discovery offers a new gateway for producing robust and hollow microspheres made of thin 2D nanomaterials to expand their applicability in various fields.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Selective photocatalytic oxidation of 5-Hydroxymethylfurfural to 2,5-Diformylfuran by Au ion exchanged CdS nanowires under Aerobic and Anaerobic conditions

Jeong Eun Kim, Hyun Sung Kim*

Department of Chemistry, Pukyong National University, Korea

5-hydroxymethyl furfural(HMF) obtained from biomass can be converted to 2,5-diformylfuran(DFF), a valuable chemical intermediate. However, the typical HMF oxidation process is required energy consuming process such as high temperature and oxygen pressure. Herein, we have fabricated Au_2S decorated CdS nanowires (denoted as Au_2S@CdS NWs) by a simple ion exchange method and applied as heterostructure photocatalyst system for HMF oxidation under mild conditions. Under visible light irradiation, the photocatalytic performance of Au_2S@CdS NWs significantly enhanced compare with pristine CdS NWs, in which Au_2S(0.25 %)@CdS NWs achieved the high DFF yield(~95 %) for 4 hour reaction time. This result means that the heterogeneous interface formed between CdS NWs and Au_2S promotes the separation efficiency of photogenerated charges, which lead to high catalytic activity. Moreover, Au_2S(0.25 %)@CdS NWs worked well for HMF conversion to DFF under both anaerobic and aerobic conditions. To investigate each reaction mechanism, a series of control experiments and characterization were conducted. Consequently, we found that the photogenerated hole directly oxidized HMF to DFF under anaerobic conditions, and the $^1O_2$ produced from oxygen is the active species for HMF conversion to DFF under aerobic conditions.

Poster Presentation : **INOR.P-5**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tunable Selectivity of Photocatalytic Benzyl Alcohol Transformation over Ag-ion-exchanged CdS Nanowires

Seo Jin An, Hyun Sung Kim*

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Existing methods for the photocatalytic transformation of aromatic alcohols into value-added products via C–C cross-coupling are inefficient and insufficiently selective. Herein, a series of cadmium sulfide nanowires (CdS NWs) loaded with Ag_2S (denoted as Ag_2S@CdS NWs) are constructed via a simple Ag^+ exchange protocol for the photocatalytic transformation of benzyl alcohol. Ag_2S@CdS NWs are decorated on the surface of CdS NWs, forming a heterogeneous interface between the Ag_2S and CdS NWs (002) planes, which enhances the photocatalytic performance of the nanowires in the transformation of benzyl alcohol to C–C coupling products or benzaldehyde. Notably, the product of the photocatalytic reaction is dependent on the amount of Ag^+ ions exchanged: with an Ag^+ exchange of less than 5 mol%, the C–C coupling product is obtained with >90% selectivity and >95% transformation yield. Conversely, with an Ag^+ exchange of 7 mol%, benzaldehyde is obtained with >90% selectivity and >90% transformation yield. Thus, the selectivity toward specific products in the photocatalytic transformation of benzyl alcohol over Ag_2S@CdS NWs is controlled by varying the amount of exchanged Ag^+ ions.

Poster Presentation : **INOR.P-6**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Introduction of the supramolecular crystallography beamline and software

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Beam Operation Team, Pohang Accelerator Laboratory, Korea

The BL2D-SMC beamline supports various techniques for the structural analysis of crystalline materials, and allows the measurement of supported high-flux X-ray with diverse wavelength range from 1.5 to 0.6 Å, and easy changeable temperature with 85 to 500K as a Cryojet 5 instrument. The diffraction data is collected by Rayonix MX225HS CCD detector with high precision Goniostat, and configuring a 10G network system enables a structural change experiment of a new single crystal through acceleration experiments. These devices can be easily used by user own through beamline software (BL2D-SMDC) In this poster, we explain the BL2D beamline at Pohang Light Source II

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Thin Silica Coating on Living Cell Membranes for Chemical and Biological Cascade Reactions.

Jeong Sang Oh, In Su Lee*

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

Inspired by nature, we aimed to create a hierarchical inorganic structure around living cell membranes like a functional jacket. The structure, consisting of metal catalysts within a thin silica layer, would allow efficient communication between chemical and biological reactions by shuttling products from one compartment to another, facilitating a programmable sequence of cascade reactions. The structure, made of ultrathin silica tiles containing metal catalysts, had minimal impact on the viability and metabolism of the living cells and demonstrated efficient catalytic performance in synthesizing various chemicals through one-pot two-step cascade reactions. This work opens the possibility for sustainable and customizable nanobiohybrid catalytic platforms that combine the natural biocatalytic capabilities of living cells with metal-catalyzed chemical reactions.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **INOR.P-8**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The Synthesis of Colloidal Silicon-Based Hollow Nanostructures through Solid State Reaction and their Bio-Application

Jeonghun Choi

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Despite of tremendous application potential, controlling the fragile Si nanostructures such as hollow-porous thin nanoshells under high-temperature solid-state reactions(SSR) is a synthetic challenge. In the present work, we introduce a SSR-guiding stratum, an embedded nanospace containing catalytic metal-silicide at a predetermined radial distance inside silica nanosphere to guide and confine the preferable growth of Si product-layer well-segregated from the rest of the volume as a result of stratum-directed phase separation process. This strategy synthesized M/Silicon (Si)-based hollow porous nanostructures (M/Si-HPNSs, M = Pd, Pt etc.) from < 100 nm silica NPs with high structural preservation under high temperature MTR conditions. The pre-constructed M-silicide stratum decided the location of newly emerging Si phase while the evolving MgO phase acted as cast, protected the HPNS during high-temperature thermal conversion and resulted to the thin porous shell of M/Si-HPNS. Due to the well-protected self-confinement, M/Si-HPNSs were conveniently dispersed as colloidal solutions in bio-relevant media, exhibiting the characteristic photoluminescence, cargo loading, and photocatalytic properties and were easily internalized inside the living cells for biorthogonal catalysis applications.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Reactions of dialkyl Pd(II) and Pt(II) complexes with organic tetrazole-thiones to afford corresponding new tetrazole-thiolato complexes

HyoungSoon Kwon, Eunji Lee, Yong-Joo Kim*

Department of Chemistry, Gangneung-Wonju National University, Korea

Tetrazole derivatives are biologically active compounds and particularly transition metal tetrazole-thiolates are attractive materials for corrosion inhibitors. In this work, we attempt formation of new alkyl, aryl, and hydrido tetrazole-thiolato Pd(II) and Pt(II) complexes from direct reactions of transition metal alkyls or zero-valent complexes with organic tetrazole-thiones {S=[C{HN4(R)}]. Reactions of dialkyl Pd(II) or Pt(II) complexes and zero-valent Pd (or Pt) complexes with organic tetrazole-thiones afford corresponding tetrazole-thiolato M(II) complexes at room temperature or thermal conditions, depending on the organic substituents. Treatments of the bis(tetrazole-thiolato)Pd(II) complexes with allyl bromide or acidic halides for organic tetrazole-sulfides are examined. We further investigate small molecule insertion of organic isocyanides into the isolated Pd(II) or Pt(II) tetrazole-thiolates.

Poster Presentation : **INOR.P-10**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Formation of Two-Dimensional Metal-Organic Frameworks Synthesized by Dicarboxylic Acids with Different Coordination Abilities

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Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[1]*Korea Basic Science Institute, Korea*

Here, we report the crystal structural differences of two Zn(II) metal-organic frameworks (MOFs, **1** and **2**) synthesized by dicarboxylic acids with different functional groups. The dicarboxylic acids used in the synthesis are 1,3-benzenedicarboxylic acid (H_2*m*-bdc) and 5-aminobenzene-1,3-dicarboxylic acid (H_2abdc). The yellow block-shaped crystals [Zn(*m*-bdc)(bpeb)]·DMA (**1**) were obtained under a solvothermal reaction using dimethylacetamide (DMA) with a mixture of Zn(II), 1,4-bis[2-(4′-pyridyl)ethylene]benzene (bpeb), and H_2*m*-bdc. MOF **1** is a two-dimensional (2D) layered structure in which a chain consisting of Zn(II) cation and *m*-bdc is bridged by two bpeb ligands. The molecular formula of the yellow block crystal synthesized with abdc is [Zn(abdc)(bpeb)] (**2**), and the synthesis conditions excluding carboxylic acid are the same as those of MOF **1**. MOF **2** is a 2D bilayered structure in which two layers consisting of coordination bonds of Zn(II) cations and abdc are bridged by bpeb ligand. In MOF **1**, two -COOs of *m*-bdc participate in the coordination bond to form a 1D chain. On the other hand, abdc of MOF **2** has three coordination bond sites with two -COOs and one -NH_2, which forms a layer by coordination bonding with Zn(II) cations. According to Schmidt's Criteria,[1] when double bonds of olefin ligands in the crystal structure are aligned closely within 3.6 Å to 4.1 Å can form cyclobutane ring by irradiation of UV. The distance between the double bonds of the adjacent bpeb in the structure of **1** is 3.8 Å. Therefore, MOF **1** is expected to have photoreactivity. MOF **2** is not expected to be photoreactive because the double bond distance of the bpeb aligned in parallel is 7.7 Å. The details will be presented and discussed in the poster.

Reference

[1] G. M. J. Schmidt, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-11**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ligand functionalization of defect-engineered Ni-MOF-74

Seonghwan Lee, Seung Bin Baek[*], Myoung Soo Lah[*]

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Incorporating functionality into the framework of metal–organic frameworks (MOFs) has attracted substantial interest because the physical and chemical properties of MOFs can be tuned by functionalizing pores. The ligand functionalization of MOF-74 is challenging because of its pristine organic ligand and framework structure. Herein, we report a series of ligand-functionalized Ni-MOF-74 derivatives synthesized by defect engineering using a mixed-ligand approach. Defect generation and ligand functionalization of Ni-MOF-74 were simultaneously achieved by incorporation of fragmented organic ligands such as 5-formylsalicylic acid, 3-hydroxysalicylic acid, 2-hydroxynicotinic acid and 5-hydroxy-1H-benzimidazole-4-carboxylic acid. The resulting defect-engineered Ni-MOF-74 derivatives maintained relatively good crystallinity up to fragment incorporation levels of ～20% and exhibited modified permanent porosity and CO2 adsorption properties depending on the functional groups and defect concentrations in the framework.

Poster Presentation : **INOR.P-12**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Sandwich-structured $Na_2Ti_6O_{13}$/rGO Composite as a High-Performance Anode for Sodium-Ion Batteries

Jungwook Song, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Sodium-ion batteries (SIBs) have the potential to be a cost-effective and sustainable solution for large-scale energy storage systems (ESSs) due to the abundance of sodium reserves. $Na_2Ti_6O_{13}$ has been considered as a suitable candidate for use as an anode material in SIBs owing to its environmental friendliness, low cost, and excellent cycling stability. Despite its advantages, $Na_2Ti_6O_{13}$ has intrinsic limitations such as low theoretical capacity (~50 mAh g^{-1}) and electrical conductivity. To overcome these obstacles, a sandwich-structured $Na_2Ti_6O_{13}$/rGO (NTO/rGO) composite was synthesized through a liquid-phase exfoliation and restacking method using electrostatic interactions. The NTO/rGO composite showed remarkable improvement in both reversible discharge capacity and cycle stability. In comparison to bare $Na_2Ti_6O_{13}$ with a discharge capacity of 20.1 mAh g^{-1} after 500 cycles, the NTO/rGO composite displayed a discharge capacity of 176.8 mAh g^{-1} at a current density of 0.1 A g^{-1} and a voltage range of 0.01-2.5 V. Furthermore, the NTO/rGO||$Na_3V_2(PO_4)_3$ full cell was assembled, discharging an energy density of 228.9 Wh kg^{-1}_{anode} with a power density of 220 W kg^{-1}_{anode} after 100 cycles in a voltage range of 1.0-4.0 V.

Poster Presentation : **INOR.P-13**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mn-doped FeOF wrapped by graphitic carbon as a cathode material for sodium-ion batteries

Ayesha Qayyum, Jongsik Kim*

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Sodium-ion batteries (SIBs) are an attractive candidate as alternatives to LIBs predominantly employed for energy storage due to their low cost and abundance. Iron oxyfluoride (FeOF) is a promising high-capacity conversion typed cathode material for SIBs, due to its large theoretical capacity of 885 mAh g^{-1}, and abundance, and eco-friendliness of Fe. However, FeOF cathode has low energy efficiency, large volume variation, poor cycling stability and rate capability, which limit their application for SIBs. In this work, for the first time, Mn doped FeOF was synthesized via solvothermal method with various manganese contents ($Fe_{1-x}Mn_xOF$, x= 0.01, 0.03, 0.05, and 0.1). $Fe_{0.95}Mn_{0.05}OF$ exhibits good cyclic performance as compared to bare FeOF with a discharge capacity of 258.4 mAh g^{-1} and a fading rate of 0.22% after 100 cycles at 100 mA g^{-1} in a 1.2-4.0 V. In addition, we utilized citric acid as both chelating agent and carbon source in the synthesized $Fe_{1-x}Mn_xOF$ to enhance the electrochemical property in SIBs.

Poster Presentation : **INOR.P-14**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Compromise between Conflicted Spatial-Arrangements of Two Organic Linkers within MOFs

Gihyun Lee, Sujeong Lee, Moonhyun Oh*

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The structural features of metal–organic frameworks (MOFs) play a vital role in determining their properties and applications, and thus the control of MOF's structure is critical to develop superlative MOFs. However, to date, only a few knowledge have accumulated on fine control of MOF structures. Herein, we report a strategy for fine tuning MOF structures based on adjusting the competitive influences of two organic linkers within an MOF. Depending on the incorporated amounts and relative contributions of two organic linkers, which have different spatial-arrangement preferences within an MOF structure, the MOFs are rationally designed to have specific structures.

Poster Presentation : **INOR.P-15**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Porous Pt@UiO-66 Composite for Efficient Catalytic Reaction

Hyunjeong Oh, Sojin Oh, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The development of porous composites containing catalytically active nanoparticles is important to improve the catalytic activity and longevity of nanocatalysts. Herein, we demonstrate the confined incorporation of active metal nanocatalysts within a metal–organic framework (MOF) and its efficient catalytic activity in the reduction of organic pollutants. UiO-66-based porous composite (Pt@UiO-66) containing well-dispersed metal nanoparticles is prepared from one-step thermal treatment of UiO-66/Pt2+. The critical features of Pt@UiO-66, such as well-dispersed nanocatalysts, well-developed pores, and characteristic surface charges, result in its efficient catalytic activity.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis, molecular magnetism, and catalysis of iron(III) complexes of 3-((2-hydroxyethyl)(pyridin-2-ylmethyl)amino)propan-1-ol

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Recently, we are interested in multidentate ligands containing hydroxyl and pyridine groups which can form monomeric and dinuclear complexes. Metal complexes, especially, iron(III) ions with polydentate ligands, could display significant coordination chemistry, magnetic properties, and catalytic activity. Here, two iron(III) complexes were reported, i.e., [(Hpmiep)Fe(NO3)]2(NO3)2] (1) and [Fe(Hpmiep)(NCS)2] (2) were synthesized through the reaction of FeSO4·7H2O/Fe(NO3)3·9H2O in methanol, respectively, with 3-((2-hydroxyethyl)(pyridin-2-ylmethyl)amino)propan-1-ol (H2pmiep) and potassium thiocyanate. The complexes were investigated by single-crystal X-ray diffraction, catalysis, and magnetochemistry. In complex 1, one iron(III) ion was bonded with a mono-deprotonated Hpmiep ligand and a nitrate ion. The two iron(III) ions within the dinuclear unit were connected by two ethoxy groups with an inversion centre. In complex 2, an iron(III) ion has a distorted octahedral structure that is bonded by two thiocyanate anions and one Hpmiep ligand. Complex 1 showed significant antiferromagnetic couplings through the bridging ethoxy groups between the iron(III) ions, whereas complex 2 has a very weak antiferromagnetic interaction. Interestingly, complex 1 showed efficient catalytic activities toward various olefins with modest to excellent yields. In this poster, we will discuss the synthesis, crystal structure, magnetism, and catalytic activities of iron(III) complexes.

Poster Presentation : **INOR.P-17**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

IZCp and PZCp: redox non-innocent cyclopentadienyl ligands as electron reservoirs for sandwich complexes

Hyeonjeong Choi, Eunsung Lee*

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

A long-sustained effort of systematic steric and electronic modification of cyclopentadienyl (Cp) ligands has enabled them to find wide-ranging valuable applications. Herein, we present two new Cp ligands: imidazolium- and pyrrolinium-substituted zwitterionic Cps (IZCp 1a and PZCp 1b), whose key utility is redox non-innocent ability to participate cooperatively with the metal center in redox reactions. Thus, the Mo(0) half-sandwich (3a, 3b) and Ru(II) sandwich ([4a]PF6, [4b]PF6) complexes of IZCp and PZCp were prepared, fully characterized, and showed by cyclic voltammetry reversible one-electron reduction at E1/2 potentials ranging from −1.7 to −2.7 V vs. Fc/Fc+. These values are extremely low and have not been observed with other Cp ligands due to the instability of the reduced complexes. DFT calculations for the reduced derivatives with IZCp and PZCp: $[3a]^-$, $[3b]^-$, 4a, and 4b showed their spin densities to be highly delocalized over their ZCp ligand moieties (70%–90%). EPR analysis of the isolated K[3b] and 4b also indicated a high degree of ligand-localized radical character. Thus, the IZCp and PZCp ligands act as electron reservoirs to sustain these Mo and Ru complexes in highly reduced states. At the same time, the CO stretching frequencies of K[3b]: νCO 1871, 1748, and 1699 cm−1, rank the $[PZCp]^-$ ligand as the strongest electron-donating Cp ligand among the reported CpMo(CO)3 derivatives, whose νCO > 1746 cm−1. In addition, these redox non-innocent Cps were obtained in high yields and found to be practically air- and moisture-stable, unlike typical Cps.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Double-doping Effect and Phase-transition of the Thermoelectric $Ca_{3-x}Sr_xAl_{1-y}Zn_ySb_3$ System

Dong Hwan Seo

Chungbuk Natioanl University, Korea

Thermoelectric (TE) materials and devices show great potential in addressing energy loss and energy crisis issues by converting wasted heat into electricity. The Zintl phase 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 and results in a high zT value. Among the various Zintl phase thermoelectric compounds, the A_3MPn_3 (A = Ca, Sr, Ba, Eu; M = Al, Ga, In; Pn = Sb, As, P) system was reported to have five different structure types, including the orthorhombic Ca_3AlAs_3(*Pnma*), Ba_3AlSb_3(*Cmce*), Ba_3GaSb_3(*Pnma*), the monoclinic Sr_3GaSb_3($P2_1/c$), and Rb_3TiO_3($P2_1/c$) types. In particular, Ca_3AlSb_3 is known to have the Ca_3AlAs_3-type structure and is composed of infinite chains of corner-sharing $AlSb_3$ tetrahedra. Sr_3AlSb_3 has the Ba_3AlSb_3 structure type and is composed of edge-sharing $[Al_2Sb_6]^{12-}$ pairs that form ribbon shapes. Both series have extremely low thermal conductivity due to their complex structures and p-type characteristics.In this work, a series of synthesis for the $Ca_{3-x}Sr_xAl_{1-y}Zn_ySb_3$ system induced a change from Ca-type to Sr-type by replacing Ca with Sr, and at the same time it lowered the thermal conductivity through the size difference between the two ions. In addition, the Al atom was doped by the Zn atom to increase the p-type characteristics of both structure types, which result in inducing better physical properties. The title compounds were synthesized by arc-melting and Pb-metal flux method, and their crystal structures were characterized using powder and single-crystal X-ray diffractions. The electronic structure of the title compounds was studied using theoretical calculations with the TB-LMTO method, and the resulting density of states and band structure were analyzed in detail. The electrical transport properties including electrical conductivity and Seebeck coefficients were also measured.

Poster Presentation : **INOR.P-19**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 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

Chungbuk Natioanl University, Korea

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 characteristics, a series of $Ba_{1-x}Eu_xZn_2Sb_2$ ($0.04(1) \leq x \leq 0.15(1)$) compounds has been synthesized by both the Nb-tube and molten Pb-flux method. Large bar-shaped single crystals were successfully obtained, and their isotypic crystal structures were characterized by the powder and single-crystal X-ray diffraction analysis. Based on the crystal structure analysis, 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 indicated more metallic properties. The thermal conductivity, electrical conductivity, and Seebeck coefficient of $Ba_{1-x}Eu_xZn_2Sb_2$ (x = 0.1, 0.15) were also carefully studied. The lowest thermal conductivity of 0.42 W/m·k is obtained for the $Ba_{0.85}Eu_{0.15}Zn_2Sb_2$ sample at 471K. The highest zT of ca. 0.44 is obtained for the $Ba_{0.85}Eu_{0.15}Zn_2Sb_2$ sample at 772K. As intended, the thermal conductivity was lowered, but the power factor was also reduced, so the zT value did not change as much as we expected.

Poster Presentation : **INOR.P-20**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Experimental and Theoretical Studies for the Zintl Thermoelectric$Ca_{3-x}Yb_xAlSb_3$ System

Junsu Lee

Department of Chemistry, Chungbuk Natioanl University, Korea

Thermoelectric (TE) materials and devices have great potential to reduce energy issues since they can convert wasted heat from various heat sources into electricity based on the Seebeck effect. Thermoelectric performance is defined as the dimensionless figure-of-merit $ZT = \sigma S^2T/\kappa$ (σ: electrical conductivity, S: Seebeck coefficient, T: absolute temperature, κ: thermal conductivity). The Zintl phase is one of the most promising candidates for TE applications due to its complex crystal structure and semiconducting property. Several examples of these Zintl TE materials include the $A_{14}MSb_{11}$ (A = Ca, Yb; M = Mn, Al), AM_2Sb_2 (A = Ca, Sr, Ba, Eu, Yb; M = Zn, Cd), A_2CdSb_2 (A = Ca, Yb, Eu), A_5M2Pn6 (A = Ca, Yb; M = Al, In, Pn = Ge, Sb,), and A_3MPn_3 (A = Ca, Sr, Ba, Eu ; M = Al, Ga, In; Pn = Sb, As, P). In particular, the Ca_3AlAs_3-type structure is one of the several Zintl 3–1–3 compositional families including the Ba_3AlSb_3, the Ba_3GaSb_3, the Sr_3GaSb_3, and the Rb_3TiO_3-type phases. The Zintl 3–1–3 compositional families involve the MPn_4 tetrahedra in common, and it shows slightly different types of structures depending on the arrangement of MPn_4 tetrahedra. The Ca_3AlSb_3 is a semiconductor with low thermal conductivity, so it has a high potential as a TE material. In this work, we explored the cation-substitution effect on the crystal structure, electronic structure, and physical properties in the $Ca_{3-x}Yb_xAlSb_3$ ($0 \leq x \leq 0.81(1)$) system. Four title compounds were synthesized by both the arc-melting method and the Pb-metal flux reaction method. Both powder and single-crystal X-ray diffraction analysis characterized their crystal structures. The particular cationic site-preference at the three available cationic sites is thoroughly studied by theoretical investigations using the electronic-factor criterion based on QVAL. To further understand the electronic structure of the title compounds, a series of theoretical calculations using the tight-binding linear muffin-tin orbital method was performed, and the resultant density of states, band structure, and electron localization function analyses were carefully conducted. Physical properties including electrical conductivity, Seebeck coefficient, and thermal conductivity of the quaternary title compound $Ca_{2.19(1)}Yb_{0.81}AlSb_3$ were examined and compared to the ternary Ca_3AlSb_3 as a reference.


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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and Electrochemical Characterization of 1,1-DialkylBenzosilole

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-Dialkylbenzosilole were produced through reactions of the prepared 2,2-dibrombiphenyl with *n*-butyllithium and dichlorodialkyl(R = Et, *n*-Hex, phenyl) silane in THF solvent, respectively. After the reaction was completed, the lithium salts were removed by washing with a dilute HCl aqueous solution. The crude product was extracted with dichloromethane (DCM) and ether, and further purified by recrystallization in petroleum ether. 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, 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-22**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and structural characterization of silole derivatives

Se yeon Park, Young Tae Park[1,*]

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

1,1-Dialkyl(R = Et, *iso*-Pr, *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles were prepared by the intra-molecular substitution reaction of 1,1-dialkyl (R = Et, *iso*-Pr, *n*-Hex)-1,1-di(phenylethynyl)silanes with treatment of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and *N*-bromosuccinimide in situ. Two bromine groups of the prepared siloles were substituted with two trimethylsilylethynyl groups using trimethylsilylacetylene (TMSA) under the solvent of diisopropylamine and catalysts such as palladium chloride, copper iodide, and triphenylphosphine, of which 1,1-dialkyl (R = Et, *iso*-Pr, *n*-Hex)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles were yielded, respectively. 1,1- Dialkyl (R = Et, *iso*-Pr, *n*-Hex)-2,5-diethynyl-3,4-diphenyl-siloles were successfully prepared by desilylation reactions of 1,1-dialkyl (R = Et, *iso*-Pr, *n*-Hex)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles with potassium carbonate (K_2CO_3) and co-solvent of tetrahydrofuran (THF) / methanol, respectively. After the reaction was finished, potassium carbonate was removed by washing with dilute HCl aqueous solution. The crude product was extracted with dichloromethane (DCM), and further purified by recrystallization in hexane. The obtained product was soluble in usual organic solvents such as tetrahydrofuran and dichloromethane. All the prepared materials were characterized by ^{1}H, ^{13}C, ^{29}Si NMR, IR, TGA, and UV-Vis spectroscopic methods. The bend gaps of the siloles were analyzed through a Gaussian program.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-23**

Inorganic Chemistry

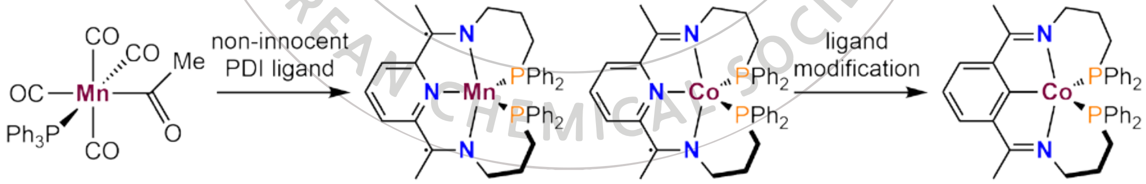
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of a Cobalt(I) Carbonyl Hydrosilylation Catalyst

Sangho So, Ryan J. Trovitch[1,*], Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*School of Molecular Sciences, Arizona State University, United States*

Hydrosilylation of unsaturated C=C/O functionalities is an important and useful reaction for forming Si–C and Si–O bonds. This chemistry involves multi-electron processes, including oxidative addition to the metal center for activating the Si–H moiety and reductive elimination to afford the hydrosilylated product. Typically, noble transition metal catalysts such as Ru, Rh, or Ir complexes are often employed due to their ability to undergo these multi-electron processes. Owing to their high cost and limited availability, chemists have attempted to develop Earth-abundant metal catalysts. Herein, we introduce recent work on the development of a carbonyl hydrosilylation catalyst through a first-row transition metal. We also provide a plausible mechanism for this reaction.



Cutler's Mn
TOF = 27.2 min^{-1}
for acetone

MnPDI, CoPDI
TOF = 1,280 min^{-1}
for benzaldehyde (MnPDI)

CoADI
TOF = 19,800 min^{-1}
for benzaldehyde

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Optical Microscopy of Light-Driven Chemical Reactions in a Single Nanocatalyst

Yongdeok Ahn, Daeha Seo[*]

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

Due to their high absorbance in the visible region, i.e. surface plasmon resonance, plasmonic metals such as Au and Ag have been seen as attractive materials for heterogeneous photocatalysts (SPR). Although Au nanoparticles do not, on their own, exhibit particularly impressive catalytic performance in comparison to standard semiconductor photocatalysts, they do greatly enhance the catalytic activity of the semiconductor with which they are in contact. The mechanism for hot electrons created by interband excitation, and their contributions on the catalysts, are not well known, although several methods based on SPR excitation have been proposed to explain how Au contributes to the enhancements. The observation and quantification of electron transfer in heterogeneous catalysis remains challenging using traditional techniques. In this study, a combination of catalytic materials and excitation wavelengths was devised to investigate the electron transfer between plasmonic materials and semiconductors. To monitor and activate the catalytic process, we employed total internal reflection fluorescence (TIRF) microscopy in conjunction with a plasmonic/semiconductor (Au/Cu_2O) hybrid nanoparticle. Since, TIRF microscopy allows the selective activation and observation of the light-driven reaction at single-particle level, we revealed the important kinetic constants, which were obscured by complex reaction factors in conventional methods, e.g. adsorption, desorption and ensemble averaging. Additionally, we determined the relative contribution of hot electrons generated via SPR and interband excitation, and we suggested a pathway for electron transfer from the sp band of Au to the valence band of Cu_2O.

Poster Presentation : **INOR.P-25**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 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

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. The TE material can be made using the Zintl phase, which is easy to dope because it has a semiconductor property and a 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. Previous study shows 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 balance the overall charge structurally. 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 *p*-dopant to mix Cu^+ with Zn^{2+}, not only did the effect of Ca/Yb mixing, but the hole carrier concentration increased to obtain an overall synergy effect. A series of compounds in the $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ ($0.5\leq x\leq 4.5$; $0.05\leq y\leq 0.2$) system was synthesized using the conventional high-temperature method and the Pb-metal flux method, and we confirmed that the single-crystal with the bar-shaped grew nicely. Crystal structures were characterized by both powder X-ray diffractions and single-crystal X-ray diffractions. Theoretical calculations were also conducted through the tight-binding linear muffin-tin orbital method, and the DOS, COHP, and band structure of the three title compounds were analyzed to understand the electronic structure.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Hierarchical Mesoporous Silica Nano Spheres and Adjusting Their Structural Characteristics

Ji Myeong Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Porous materials, especially nano-sized porous materials have been studied and evaluated for decades due to their large surface area, pore volume and applicability to various areas. Particulary, mesoporous silica nano materials have received a lot of attention due to their facile synthesis mechanisms and stability. Hierarchical Mesoporous Silica(HMS), one of the mesoporous silica structures, is highly competitive since its three-dimensional pore channel structure and adjustable pore size. By varying factors, such as templates and catalysts, HMS was synthesized by controlling its particle size and pores. Scanning Electron Microscope(SEM) and Transmission Electron Microscope(TEM) were used to verify its morphological properties. N_2 adsorption-desorption measurements were used to examine its pore characteristics. Fourier transform infrared(FT-IR) spectroscopy was used to check the residues were well removed. The synthesized HMS is expected to be used in various areas by functionalization or its framework structure itself.

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

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Platinum Nanocubes With Atomic Transition Metal Decoration to Improve The Electrochemical Ammonia Oxidation Reaction Performance

Saehyun Park, Sang-Il Choi*

Department of Chemistry, Kyungpook National University, Korea

The continuous rise in carbon dioxide emissions is the primary contributor to the global warming crisis. To tackle this problem, numerous studies are being carried out, and one promising solution is the use of an ammonia fuel cell or an ammonia electrolytic cell. Ammonia is a carbon-free material that has a higher energy density, is easier to handle and transport than hydrogen, and is considered eco-friendly because it does not release carbon dioxide as a byproduct, unlike traditional systems that use organic matter as a reactant. However, the stability of the anodic reaction ammonia oxidation reaction (AOR) is an issue as the catalyst that facilitates AOR is susceptible to poisoning from N-species intermediates (Nads, NOads). One solution to solve this poisoning phenomenon is to introduce a transition metal into the catalyst. Although the exact cause of the heightened resistance to poisoning remains unknown, many reports indicate that stability is increased when transition metals are added. In our research, we introduced various transition metals (Fe, Co, Ni, Cu, Zn, Ru, Rh) at the atomic level onto a platinum nanocube and applied it to the ammonia oxidation reaction.

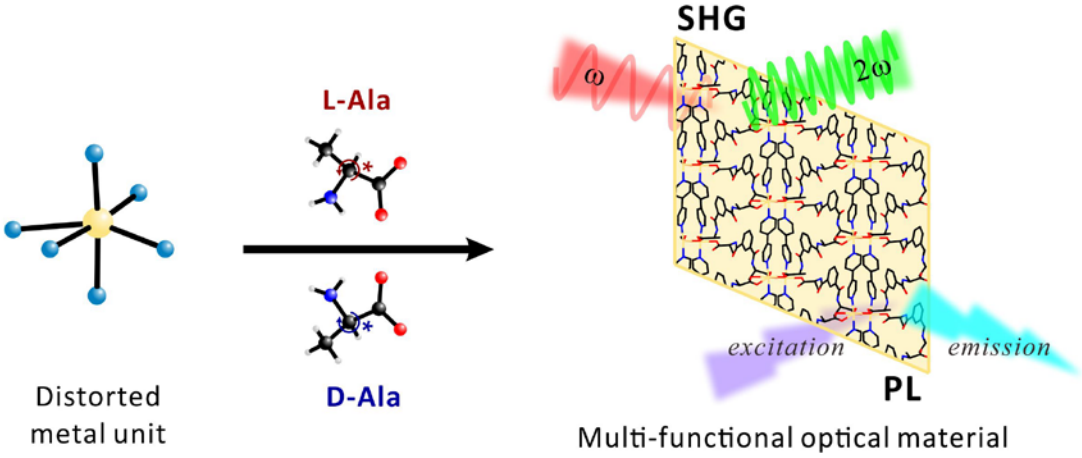
Poster Presentation : **INOR.P-28**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Homochiral coordination polymers: a strategy for efficient synthesis of crystalline materials with noncentrosymmetric structures and unique properties

Jihyun Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Crystalline materials with noncentrosymmetric (NCS) structures have garnered attention in the industrial field owing to their useful properties such as piezoelectricity, ferroelectricity, and second-harmonic generation (SHG). Asymmetric building units are utilized to induce NCS structures; however, arranging them without an inversion center is a challenging issue. We found that introducing homochiral organic molecules is a great strategy to systematically and efficiently synthesize crystalline materials with NCS structures. In this work, a series of homochiral coordination polymers (HCPs) were synthesized using two kinds of ligands, an alanine-based dicarboxylate ligand and a pillar-like bipyridine ligand. The crystal structures of the target compounds were determined by single crystal X-ray diffraction. For example, compound 1 crystallized in the triclinic chiral space group, $P1$, with the aid of the chiral ligands. The unique three-dimensional structure was formed via intermolecular interactions such as hydrogen bonds and π-π stacking. The HCPs with NCS structures exhibit moderate SHG efficiencies of ca. 1.5–2.1 times that of KH_2PO_4. In addition, compound 1 exhibits an unusual excitation wavelength-dependent photoluminescent phenomenon owing to interligand charge transfer. We will present the synthesis, structure determination, and optical properties of the HCPs.


SHG
ω
2ω
L-Ala
Distorted metal unit
D-Ala
excitation
emission
PL
Multi-functional optical material

Poster Presentation : **INOR.P-29**

Inorganic Chemistry

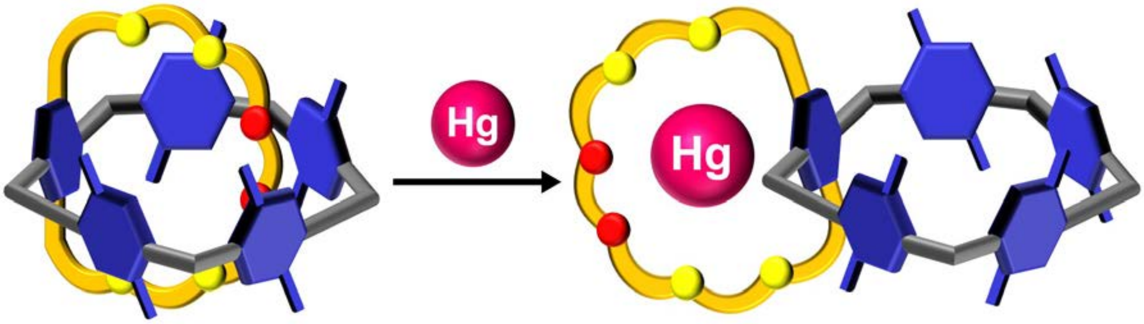
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

pseudo-Catenane Type Pillar[5]thiacrown: Planar Chiral Inversion by Mercury(II) Ion Under the Control of Anions

Yelim Lee, Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

A *pseudo*[1]catenane-type pillar[5]thiacrown (*rac*-L) having planar chirality was synthesized and the two enantiomers (*in-pS*-L and *in-pR*-L) were isolated by chiral column chromatography. We confirmed that the chiral inversion from *in-pR*-L to *out-pS*-L was triggered by mercury(ll) perchlorate and mercury(ll) nitrate. In the NMR studies, furthermore, peaks for crown ether chain of *in-pR*-L were shifted to down field area in the presence of mercury(ll) perchlorate. The observed results indicate that the conformational changes of the ligand occured from *in*-form to *out*-form by chiral inversion. Surprisingly, the negative cotton effect of *out*-form is changed to zero value as time goes on. This means that the conformation of *out*-form ligand has changed to a different conformation. In the crystal structure of mercury(II) bromide complex with *rac*-L, the mercury(II) ion exists outside the thiacrown with an exo-coordination mode and maintains the *pseudo*[1]catenane-type configuration. The structure for the mercury(II)-selective planar chiral inversion and its structural dynamics is under investigation by NMR study and DFT calculation.



Poster Presentation : **INOR.P-30**

Inorganic Chemistry

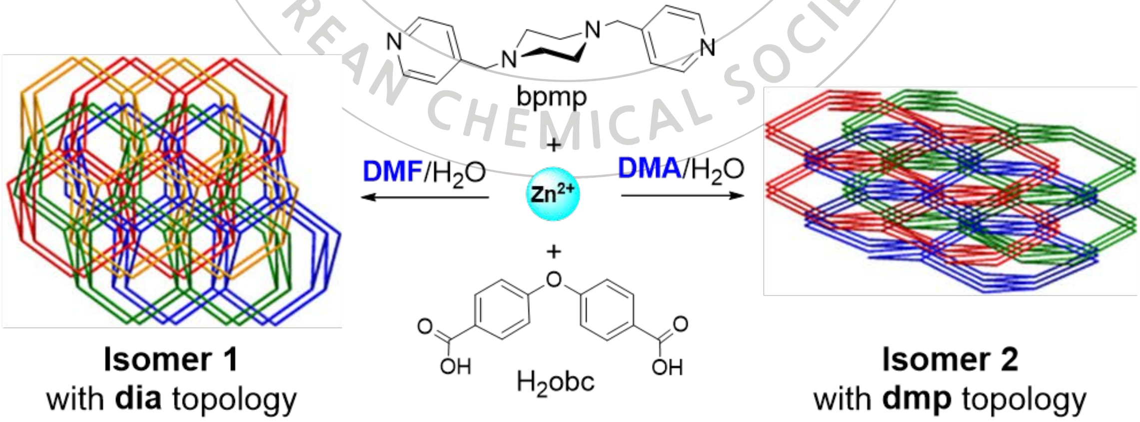
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Solvent-Dependent 3D Zn(II) Supramolecular Isomers with Different Network Topologies Based on a Flexible Dipyridyl Piperazine

Seo Hyeon Yun, Yelim Lee, Joon Rae Kim, Huiyeong Ju[1,*], Eunji Lee[*]

Department of Chemistry, Gangneung-Wonju National University, Korea
[1]*Korea Basic Science Institute, Korea*

Structural characterization and physical properties of two 3D Zn(II) supramolecular isomers (1 and 2) with different network topologies and degrees of interpenetration depending on the solvents are reported. In DMA/H_2O, solvothermal reaction of $Zn(NO_3)_2 \cdot 4H_2O$, a flexible dipyridyl ligand (bpmp, 1.4-bis(4-pyridylmethyl) piperazine), and bent dicarboxylic acid (H_2obc) afforded a 4-fold interpenetrated product, $\{[Zn(bpmp)(obc)] \cdot xSolvent\}_n$ (1) with a 4-connected dia net topology. When DMF was used instead of DMA under identical conditions, 3-fold interpenetrated supramolecular isomer $\{[Zn_2(bpmp)_2(obc)_2] \cdot xSolvent\}n$ (2) with a 4-connected dmp net topology was isolated.



Poster Presentation : **INOR.P-31**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Supramolecular Coordination Networks of Soft Metal Ions with a Sulfur-Bearing Linear Pillar[5]arene Derivative

Joon Rae Kim, Yelim Lee, Seo Hyeon Yun, Eunji Lee[*]

Department of Chemistry, Gangneung-Wonju National University, Korea

One of challenging tasks in the coordination polymer chemistry comes from how dimensional diversity might be controlled and how such behavior might be applied. We proposed a flexible linear ligand due to the free rotation of the ethylene group between donor atoms, which induces structural diversity across their respective complexes. In this work, a flexible sulfur-bearing pillar[5]arene ligand (L) was synthesized and their supramolecular coordination networks are reported. Furthermore, complexation studies of L with soft metal ions in solution and solid states are in progress.

Poster Presentation : **INOR.P-32**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Air-and Moisture-Stable Organic Radicals Derived from Oxalyl Chloride

Solhye Choe, Eunsung Lee[*]

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

It is difficult to design and make air-persistent organic radicals (APORs) because air contains a number of reactive small molecules, including water, carbon dioxide, and dioxygen. As dioxygen quickly quenches open shell compounds, it is crucial for the design of APORs to control the reactivity of organic radicals. For stabilizing radical centers, N-heterocyclic carbenes (NHCs) are advantageous due to their large substituents and low-lying empty π-orbitals. Our group recently published a study on the synthesis of 1,2-dicarbonyl radical cations that are stable against air, moisture, and heat. They have the potential for use in a variety of applications, including the creation of flexible electronics and MRI contrast agents. Therefore, it is significant to develop practical and adaptable syntheses for APORs.Herein, we explain the synthesis of two different forms of APORs using cyclic (alkyl)(amino)carbene (cAAC) and oxalyl chloride. Surprisingly, the reaction of oxalyl chloride with cAAC produced not only the expected cAAC-derived 1,2-dicarbonyl radical cation but also the previously prepared (amino)(carboxy) radical cation. The detailed synthesis and full characterization of the radical including X-ray determined structure and EPR spectroscopy will be presented.

Poster Presentation : **INOR.P-33**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Two-Dimensional Zn-MOF and Its Fluorescence and Catalytic Properties

Jongseo Kim, Seong Huh*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

A two-dimensional (2D) Zn metal-organic framework (Zn-MOF), [Zn(3-DPPy)(BDC)], with a fluorescent 1,6-di(pyridin-3-yl)pyrene (3-DPPy) and 1,4-benzenedicarboxylate (BDC) bridging linkers was prepared and structurally characterized. The mononuclear Zn(II) ion acting as a node is tetrahedrally coordinated with two 3-DPPy and two BDC linkers. The geometry of Zn(II) is a distorted tetrahedral. The Zn-MOF is a sql network structure based on topology analysis. The undulated 2D sheets of Zn-MOF tightly pack together to form a layered structure. The Zn-MOF is nonporous possibly because of the mononuclear Zn(II) node without any cluster-based secondary building units. The fluorescence measurements indicate that the maximum fluorescent signal of the 2D Zn-MOF is slightly blue shifted compared to the free 3-DPPy in solid state. Despite its nonporosity, the surface Lewis acidic sites of Zn-MOF could catalyze the transesterification of esters.

Poster Presentation : **INOR.P-34**

Inorganic Chemistry

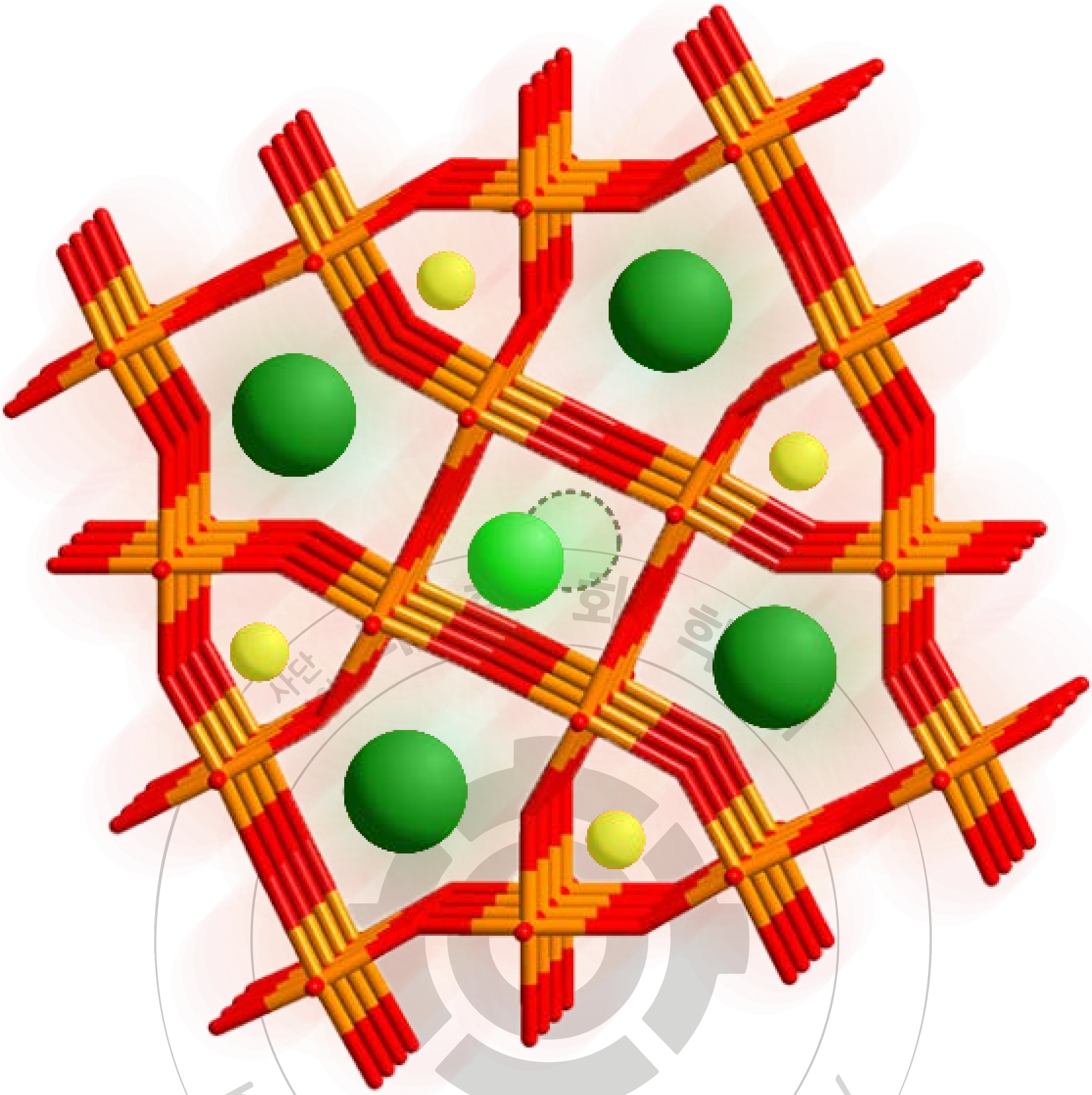
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and Characterization of a Tetragonal Tungsten Bronze with Extremely High Second Harmonic Generation Efficiency

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Recently, the discovery of solid-state materials with large polarization has drawn attention to obtain novel materials with strong second harmonic generation (SHG). Among many, polar tungsten bronze structures have proven to be perfect candidates as nonlinear optical (NLO) materials. Especially, $Pb_2K_{0.5}Li_{0.5}Nb_5O_{15}$ (30 × KH_2PO_4 (KDP)), $Pb_2(Pb_{0.15}Li_{0.7}\square_{0.15})Nb_5O_{15}$ (39 × KDP), and $Pb_{2.15}(Li_{0.25}Na_{0.75})_{0.7}Nb_5O_{15}$ (47 × KDP) reveal strong SHG responses attributed to the large polarization obtained from well-aligned NbO_6 octahedra.We have successfully synthesized a tetragonal tungsten bronze by combining second-order Jahn-Teller distortive cations through a solid-state reaction. The title compound exhibits an extremely large SHG efficiency of about 71.5 times that of KDP and displays type-I phase-matching behavior. To the best of our knowledge, the title compound has the strongest SHG efficiency among all reported NLO materials to date. In this presentation, we present the synthesis, structure, and characterization of the new tungsten bronze, along with detailed calculations.



Poster Presentation : **INOR.P-35**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Aldehydes Oxidation Reaction into Carboxylic Acids by a Manganese(III) Iodosylbenzene Complex through Electrophilic C–H Bond Activation

Hyokyung Kim, Donghyun Jeong, Jaeheung Cho*

Department of Chemistry, UNIST, Korea

The oxidation of aldehyde is one of the fundamental reactions in the biological system. Synthetic procedures and catalysts have been developed to convert aldehydes into carboxylic acids efficiently under ambient conditions. In this work, we report the oxidation of aldehydes by mononuclear manganese(III) iodosylbenzene complex, $[Mn^{III}(TBDAP)(OIPh)(OH)]^{2+}$ (1), with kinetic and mechanistic studies in detail. The reaction of 1 with aldehydes resulted in the formation of corresponding carboxylic acids via pre-equilibrium state. Hammett plot and reaction rates of 1 with 1°-, 2°- and 3°-aldehydes revealed the electrophilicity of 1 in the aldehyde oxidation. Kinetic isotope effect (KIE) experiment and reactivity of 1 towards cyclohexanecarboxaldehyde (CCA) analogues indicate the reaction of 1 with aldehyde occurs through the rate-determining C–H bond activation at the formyl group. The reaction rate of 1 with CCA is correlated to the bond dissociation energy (BDE) of the formyl group plotting linear correlation with other aliphatic C–H bonds. Density functional theory (DFT) calculations found 1 electrostatically interacts with CCA at the pre-equilibrium state in which the C–H bond activation of the formyl group is performed as the most feasible pathway. Surprisingly, the rate-determining step is characterized as hydride transfer from CCA to 1 affording an (oxo)methylium intermediate. At the fundamental level, it is revealed the hydride transfer is composed of H atom abstraction followed by a fast electron transfer. Catalytic reactions of aldehydes by 1 are also presented with broad substrate scopes. This novel mechanistic study gives better insights into metal oxygen chemistry and would be prominently valuable for development of transition metal catalysts.

Poster Presentation : **INOR.P-36**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis, crystal structure, photoluminescence, and magnetic properties of chiral lanthanide(Ⅲ) complexes showing near-IR emission

Yuri Jeong, Anh Le Ngoc Tram[1], Ihsan Ullah[2], Yoon Jung Jang[3], Kil Sik Min[*]

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Lanthanide metal complexes have attracted a great interest because they can act as molecular magnets and light-emitting materials in the field of coordination chemistry. Here we report a series of chiral lanthanide coordination complexes which show near-infrared emission. The Schiff base ligand with two chirality centers, (R,R)-N,N'-bis(3,5-dinitrosalicylidene)-1,2-cyclohexanediamine ((R,R)-H2dnsalcd), was obtained by the reaction of 3,5-dinitrosalicylaldehyde and (1R,2R)-(+)-1,2-cyclohexanediamine and further used for synthesis of four lanthanide(Ⅲ) complexes, (teaH)[Nd((R,R)-dnsalcd)2] (1), (teaH)[Ho((R,R)-dnsalcd)2] (2), (teaH)[Er((R,R)-dnsalcd)2] (3), and (teaH)[Yb((R,R)-dnsalcd)2] (4). The complexes were characterized by IR, UV-vis, photoluminescence, circular dichroism, molecular magnetism, and single crystal X-ray diffraction. Complexes 1-4 show distorted square antiprism geometry structures via coordination of four oxygen and four nitrogen atoms in two dnsalcd2- ligands and triethylammonium (teaH+) was included as cation for charge balance. Complex 1 crystallizes in the orthorhombic P212121 space group, and complexes 2-4 crystallize in the hexagonal P61 space group. All complexes showed strong light emissions in near-IR region by excitation at 380 nm and demonstrated its strong antenna effect due to the energy transfer from ligand to Ln(Ⅲ) core. The magnetic susceptibility data was plotted as χMT versus T and all complexes exhibited paramagnetic behavior. These findings provide fundamental insights into the design of efficient optical materials with enhanced luminescence properties and potential applications such as light-emitting diodes, night vision device, and telecommunication.


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Poster Presentation : **INOR.P-37**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chiral Cages Transformation and Chiral DOPA Recognition

Dongwon Kim, Kim Daeun, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of $Hg(ClO_4)_2$ with pair of C_3-symmetric chiral ligands, (1*S*,1'*S*,1"*S*,2*R*,2'*R*,2"*R*)-(benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1H-indene-2,1-diyl)trinicotinate (*s*,r-L) and (1*R*,1'*R*,1"*R*,2*S*,2'*S*,2"*S*)-(benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1H-indene-2,1-diyl)trinicotinate (*r*,*s*-L), produces a pair of chiral cages $C_4H_8O_2@[(Hg_2^{II})_3(ClO_4)_6(s,r\text{-}L)2](C_4H_8O_2)_7(H_2O)_7$ and $C_4H_8O_2@(Hg_2^{II})_3(ClO_4)_6$ $(r,s\text{-}L)2](C_4H_8O_2)_7(H_2O)_7$, respectively, via straightforward formation of the reduced Hg_2^{II} species with an inner cavity nestled by a single dioxane molecule. The pair of chiral cages are transformed into their downsized pair of cages, $[Hg^{II}_3(ClO_4)_6(s,r\text{-}L)_2]$ and $[Hg^{II}_3(ClO_4)_6(r,s\text{-}L)_2]$, respectively, in the presence of hydrochloric acid. The original chiral cages are more effective than the corresponding downsized cages for enantio-recognition of chiral 3,4-dihydroxyphenylalanine (DOPA) via the shifts of electrochemical oxidation potentials of linear sweep voltammetry (LSV) technique. Furthermore, photoluminescent spectral shifts show of the down-sized chiral cages significantly recognize chiral DOPA.

Poster Presentation : **INOR.P-38**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Outstanding catalytic efficiency of $SiF_6@Cu_2L_4$ cageshave different structures depending on crystallization time

Hyo Jeong Back, Jihun Han, Ok-Sang Jung*

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New ligand (1S,2R)-(-)-1-(nicotinamido)-2,3-dihydro-1H-inden-2-yl nicotinate and (1R,2S)-(+)-1-(nicotinamido)-2,3-dihydro-1H-inden-2-yl nicotinate (L) are synthesized by (1S,2R)-(-)-*cis*-1-Amino-2-indanol and (1R,2S)-(+)-*cis*-1-Amino-2-indanol. Self-assembly of $Cu(BF_4)_2$ with L as a bidentate N-donor in a mixture solvent including ethanol in a glass vessel. It produces new 3D-cage structures that encapsulate unexpected hexafluorosilicate (SiF_6^{2-}) anions from glassware and have different crystal structures depending on time and solvent. In the case of crystallization in a short time, discrete $SiF_6@Cu_2L_4$ cage with outside BF_4^- anions are constructed. Whereas, in a long time, SiF_6^{2-} anion-bridged $SiF_6@Cu_2L_4$ cage are constructed. In 3,5-di-tert butylcatechol oxidation reaction, anion bridged cages as heterogeneous catalysts have better catalytic efficiency than discrete cages as homogeneous catalysts. As such, the catalytic efficiency was different depending on the anion, and additionally, these chiral cages can be applied to efficient catalyst on chiral reactions.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **INOR.P-39**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

M_6L_{12} metallacycle compound have different coordinated species by transition metal

Seonghyeon An, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of $M(ClO_4)_2$ (M^{2+} = Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}) with dicyclopentyldi(pyridine-3-yl)silane (L) as a bidentate N-donor. It produces new discrete M_6L_{12} metallacycle compound. It is unique in that they are ellipsoidal. The shape, packing mode and number of coordinated molecules are different according to metal cations. The eccentricity, determined by the ratio of the major axis to the minor axis, increases in the order Cu < Mn < Zn < Co < Ni. The crystals include toluene as a solvent, which is rapidly exchanged to *o*-, *m*-, *p*-xylene on SCSC mode.

Poster Presentation : **INOR.P-40**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effect of anion and solvent system on packing mode of Cu(II) complexes

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Self-assembly of CuX_2 (X^- = OTf^-, BF_4^-, ClO_4^-) with octamethylbis(1,7-pirydiyl)tetrasiloxane (L) as a bidentate N-donor. It produces new discrete octahedral coordination complexes. All complexes have basically same ML_2 spiro shape, but their packing mode is determined by factors like anion species/size and solvent system. In the case of $[Cu(OTf)_2L_2]$ complexes, the packing mode was different depending on solvent system, even though the anions were the same. In the case of $[Cu(BF_4)_2L_2]$ and $[Cu(ClO_4)_2L_2]$ complexes, the packing mode was the same depending on solvent system, even though the anions were different.

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **INOR.P-41**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Selective Turn-on Luminescence Sensor of C_8 Aromatic Isomers in Zinc complex Using an Anthracene-based Ligand on SCSC Mode

Gyeongwoo Kim, Gyeongmin Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Here we present new ligand (9,10-bis((isoquinolin-5-yloxy)methyl)anthracene (L)) synthesized from 9,10-Bis(bromomethyl)anthracene and isoquinolin-5-ol, further used for self-assembly with $ZnCl_2$ as a bidentate N-donor. The Zn^{2+}-based complex can show selective turn-on luminescence activity for C_8 aromatic isomers (*o*-xylene, *m*-xylene, *p*-xylene) by fluorometric methods, especially for the selective sensing of *p*-xylene. Moreover, all of the C_8 aromatic isomers are adsorbed in Zn^{2+}-based metal complex on SCSC mode. Selective sensing of *p*-xylene can be explained by stronger π-π interaction between the coordinating ligand and *p*-xylene than that of other xylenes, leading to enhanced intensity of fluorescence.

Poster Presentation : **INOR.P-42**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Regulation of Matrix Metalloproteinase-2/9 as A Potent Cancer Treatment

Eungchan Kim, 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.

Poster Presentation : **INOR.P-43**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Oxovanadium(IV) mononuclear complex derivative tetradentate reduced Schiff base ligand: synthesis, crystal structure, and characterization

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[3]*College of Basic Education, Yeungnam University, Korea*

In this study, a tetradentate reduced Schiff base ligand was used to synthesize an oxovanadium(IV) mononuclear complex. The reduced Schiff base ligand (H_2L) was synthesized by the reaction of 2,2-dimethyl-1,3-propanediamine with ortho-vanillin followed by reduction with $NaBH_4$ in methanol solution and used in the preparation of heteronuclear oxovanadium(IV)/sodium(I) complex, $[VO(L)Na(CH_3COO)]$. 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 vanadium(IV) center adopts a six-coordinate distorted octahedral geometry, with oxovanadium(IV) located in the inner N_2O_2 compartment and sodium(I) located in the outer O_2O_2' compartment of the reduced Schiff base ligand. The complex was further characterized by FT-IR, UV-Vis, PL, and ERP spectroscopy, providing valuable insights into its coordination chemistry and electronic properties. These results demonstrate that the potential of reduced Schiff base ligands as effective ligands in the synthesis of metal complexes and have implications for the design and synthesis of new metal complexes for various applications including catalysis, photoluminscence, and biomedicals. The findings of this study contribute to the advancement of our understanding of the coordination chemistry of vanadium complexes and the design of new ligand systems for the synthesis of vanadium complexes with specific properties.

Poster Presentation : **INOR.P-44**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Real time observation of organic reactions at the single molecule level

Minsoo Park

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Understanding the mechanism of chemical processes is a fundamental endeavor. However, it is uncommon to analyze each stage of the reaction mechanism and the static heterogeneity of kinetics using conventional methods including mass spectrometers, 1H-NMR, and UV-vis absorption spectroscopy. A single-molecule experiment reveals the data hidden by ensembled-averaged techniques. Here, we present a reliable method for total internal reflection fluorescence microscopy that makes use of organic dyes to track each individual molecule's chemical response in real time (TIRF). We may observe the reaction process at the single-molecule level using TIRF because of fluctuations in the length of the conjugation bond and quantum yield. This technique displays optical properties of each intermediate or transition state that are typically difficult to observe in time trajectories.

Poster Presentation : **INOR.P-45**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Rotational Brownian motion of Au NR in nanoconfined region

Siwoo Jin, Daeha Seo*

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Rotational and translational Brownian motion of anisotropic nanoparticles in a fluid, where particles undergo continual random displacement and independent molecular collision, has significant attention to investigate the nanoscale rheology of their surrounding environment. However, the measurement of three-dimensional rotation is challenging due to the confusion of signal change whether it is derived from z-axis movement or rotation. Here, we observe gold nanorods (Au NRs) in a nanoconfined region with dark-field microscopy and explore rotational motion with fluctuation-based intensity analysis. In the tethered-NR model, fluctuation frequency is inversely proportional to surrounding viscosity. Also, we investigate the rotational Brownian motion in the confined model, which shows a dramatic decrease in frequency when the diameter of a vesicle is comparable to the size of Au NR. Using this technique as a viscometer, we measure the dynamic viscosity of intracellular vesicles in a reliable and reproducible manner. Our experimental observation can be extended to measure the local viscosity of complex fluids and nanoscale dynamics in various regions.

Poster Presentation : **INOR.P-46**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrocatalytic H_2 Evolution Reaction by Cobalt Complexes Using Redox-Active Ligands

JuEun Lee, Junhyeok Seo*

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

The electrochemical hydrogen evolution reaction (HER) is a sustainable method for producing dihydrogen, a promising energy source for the future. The direction of the reaction is determined by electron transfer and proton transfer. We use cobalt and 2,2'-bipyridine (Bpy), which have redox-activity, are used to regulate the molecular orbital energy level where electron transfer occurs. We also utilized different proton sources with varying pKa values to adjust the site of proton transfer. By mediating both electron transfer and proton transfer, we observed that the hydrogen evolution reaction takes place at lower energy. We attempted to determine the reaction mechanism through experimental methods and DFT calculations. This poster will explore the electrochemical proton reduction activity of Co-bpy complexes and propose a potential reaction mechanism.

Poster Presentation : **INOR.P-47**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrochemical Behaviors of Bis(dithiolene) W-oxo Complex and Mechanistic Study for Electrocatalytic H_2 Evolution Reaction

Wonjung Lee, Jaeheon Lee, Junhyeok Seo[*]

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

Dihydrogen as a sustainable energy carrier attracts research attention, and electrochemical hydrogen evolution reaction (HER) is one of the promising methods to generate hydrogen gas using electric or solar energy. Researchers have been inspired by nature to develop efficient and economic catalysts. For example, Ni, Fe, and Co complexes mimicking the active sites in hydrogenase or vitamin B12 have been developed. W/Mo contained enzyme active sites combined with redox non-innocent dithiolene ligand have been reported as other examples, but few examples are using W center for HER. We investigated the role of axial chalcogenide ligand in Bis(dithiolene) W-oxo complex for HER and discovered the unique anodic shift after the electrochemical reaction. In this poster, I will show the electrochemical behaviors of the bis(dithiolene) W-oxo complex and demonstrate the potential-controlled reaction pathways of proton reduction using DFT calculations.

Poster Presentation : **INOR.P-48**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tetrahydroxybenzoquinone-based Metal-Organic Frameworks as Long-term Antioxidants

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Free radicals produced during metabolism induce effects such as cell damage and cancer owing to their high reactivity. Although antioxidants in food products can eliminate radicals, they are expelled within a relatively short period after serving their function. In this study, we investigated the possibility of using Metal-Organic Frameworks (MOF) with antioxidants as their ligand. Metal-Organic Frameworks are polydentate polymers with repetitively coordinated ligands and metal centers. We assume that once antioxidant-based MOFs are ingested, ligands are released on a long-term basis in the process of chemical/physical disintegration. SU-101, FeTHQ, and Cu-CAT-1 were selected as a candidate for long-term antioxidant MOF in this study. To evaluate their eligibility, we set up criteria for biocompatibility, particle size, and long-term antioxidant effects. For biocompatibility, we treated cell media with various concentrations of MOF and its precursors, followed by a WST-8 assay. In addition, we stirred the MOFs in a pH 2 HCl solution and then in PBS buffer to imitate the intake path of the MOFs when introduced into the body. The particle size distribution of the particles was analyzed using TEM and ImageJ software at 12hr intervals, and the antioxidant emission during each interval was quantified using UV-vis spectroscopy. We concluded that Fe-based FeTHQ with antioxidant Tetrahydroxy-1,4-benzoquinone(THQ) as its ligand is the most effective long-term antioxidant, and its effect can last up to 7 days, with 21 times the effect of blueberry extract. Furthermore, microwave synthesis of FeTHQ was conducted to produce more suitable particles for in vivo antioxidant applications.

Poster Presentation : **INOR.P-49**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ferroelectric Nanoparticles to Improve Tumor Treating Field Effectiveness

Juhyeong Cho, Daeha Seo[1,*]

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Tumor Treating Fields (TTFields) is an innovative, non-invasive cancer treatment based on electric field. By interfering with the alignment of polar proteins such as tubulin and septin during mitosis, this therapy uses an alternating electric field to prevent the formation of mitotic spindles and contractile rings to inhibit cell division or induce apoptosis. However, in early clinical trials, the efficacy of TTFields was not superior to conventional chemotherapy. Recently, ferroelectric BaTiO3 nanoparticles (BTO NPs) were used as sensitizers to increase the efficiency of TTFields, but the mechanism is still unclear. Herein, we designed several experimental strategies to determine which properties of nanoparticles are crucial as TTFields sensitizers. We tried to verify the presence of reactive oxygen species to confirm the chemical effect of BTO NPs under an alternating electric field, but could not be detected. Moreover, we confirmed that the steric hindrance under TTFields is negligible by comparing BTO NPs with gold nanoparticles. Finally, by comparing different nanoparticles, we showed that the efficacy of TTFields combined nanoparticles is proportional to their ferroelectricity. These results help us comprehend the physical impacts that NPs on cells in electric fields can be used as critical data for developing better sensitizers in the future.

Poster Presentation : **INOR.P-50**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chiral amino acid-templated metal fluorides with large birefringence

Ahyung Jung, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Chiral amino acid-templated metal fluoride crystals, (R)-Sn and (S)-Sn, with large birefringence have been successfully grown via a slow evaporation method. The structures of the reported compounds crystallizing in the noncentrosymmetric nonpolar space group, $P2_12_12$ were determined by single crystal X-ray diffraction. Owing to the multiple hydrogen bonding interactions between protonated ligand cations and metal fluoride octahedra, the structures of the materials are considered to be pseudo three-dimensional structures. The title compounds exhibit a large birefringence value of 0.252 @1064 nm. The observed large birefringence should be attributed to the well-stacked arrangement of the planar π-conjugated benzene rings along the *b*-axis. Additionally, the birefringence is influenced by the dihedral angle between the organic ligand groups and the octahedral distortion. Ultraviolet-visible diffuse reflectance spectra and density functional theory calculations indicate that the title compounds have a large band gap of up to ca. 4.20 eV. Powder second-harmonic generation (SHG) measurements, conducted using 1064 nm radiation, reveal that the title compounds have mild SHG efficiencies.

Poster Presentation : **INOR.P-51**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and characterization of two chiral Cd-based metal-organic coordination polymers

JinSoo Koh, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Two Cd-based metal-organic coordination polymers, Cd(*S*) and Cd(*R*), have been synthesized by hydrothermal reactions. Single crystal X-ray diffraction indicates that both Cd(*S*) and Cd(*R*) crystallize in the monoclinic non-centrosymmetric polar space group, $P2_1$, (No. 4). Cd^{2+} cations are coordinated by chiral organic ligands and bipyridine, resulting in 6– and 7– coordinate environments. The coordination polymers form 1D chain structures held together by T-shaped C–H…pi interactions between the H atoms of the chiral ligand's phenyl rings and the C atoms of bipyridine. The photoluminescence spectra of Cd(*S*) and Cd(*R*) exhibit a broad emission peak in the 400–700 nm range when excited by a 390 nm. The spectra emit blue light with emission coordinates of (0.23, 0.29) and (0.22, 0.28), respectively, and decay lifetimes of approximately 0.341 and 0.378 ms.

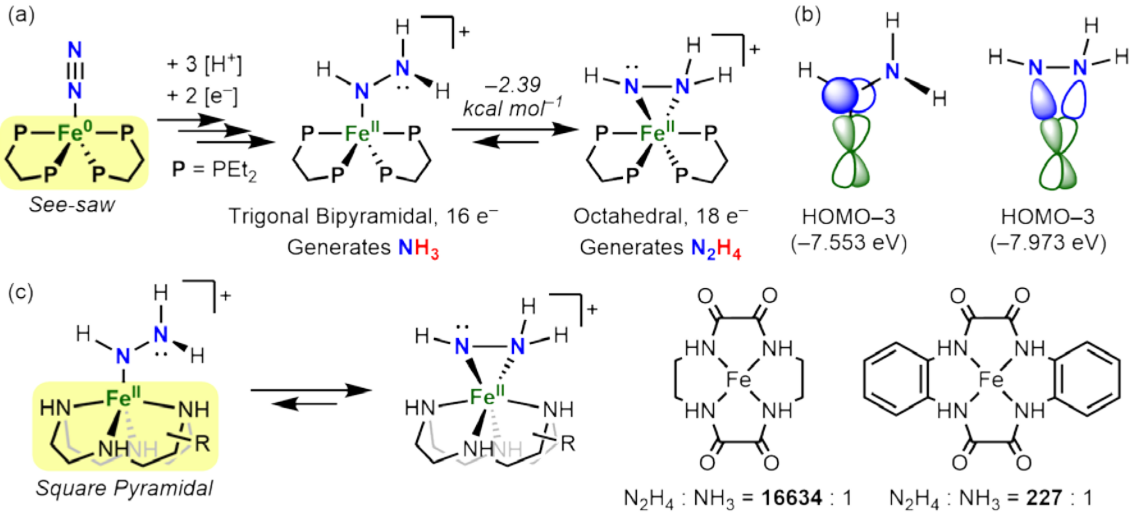
Poster Presentation : **INOR.P-52**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Understanding the Origin of Hydrazine Selectivity in Nitrogen Reduction

Seongyeon Kwon, Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Nitrogen gas serves as the primary source of nitrogen atoms, and its conversion to ammonia is a vital process that supplies nitrogen to the biosphere and chemical industry. Hydrazine is a potential product of nitrogen reduction and is actively used as an energy source due to its high energy density. However, the selective production of hydrazine presents a challenge as its formation energy is much higher than that of ammonia. In 2016, the Ashley group first reported an Iron catalyst that selectively generates hydrazine. The density functional theory calculations were carried out to understand the detailed mechanism and the origin of the selectivity. We discovered that the see-saw structure of the ligand scaffold allows the formation of an octahedral intermediate, which prevents the generation of ammonia and promotes the production of hydrazine. The stabilization of the π-bonding orbital through the isomerization is identified as the driving force behind this process. Based on this principle, we envisioned that the tetraaza-macrocyclic ligands would be beneficial for the selective production of hydrazine. Herein, we provide promising ligand candidates predicted to have high selectivity and the operating ability for hydrazine synthesis.


(a)
+ 3 [H+]
+ 2 [e−]
P = PEt2
See-saw
−2.39 kcal mol−1
Trigonal Bipyramidal, 16 e−
Generates NH3
Octahedral, 18 e−
Generates N2H4
(b)
HOMO–3
(–7.553 eV)
HOMO–3
(–7.973 eV)
(c)
Square Pyramidal
N2H4 : NH3 = 16634 : 1
N2H4 : NH3 = 227 : 1

Poster Presentation : **INOR.P-53**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

$Cd(NH_2SO_3)_2 \cdot xH_2O$ (x = 0, 2): synthesis and characterization of two cadmium sulfamates with unique structures and phase transitions

Xuefei Wang, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Two new cadmium sulfamates, namely, centrosymmetric $Cd(NH_2SO_3)_2 \cdot 2H_2O$ and noncentrosymmetric $Cd(NH_2SO_3)_2$ have been successfully synthesized. $Cd(NH_2SO_3)_2 \cdot 2H_2O$ has an infinite chain structure consisting of *trans*-$[CdO_2(H_2O)_2(NH_2)_2]$ octahedra and $[NH_2SO_3]$ units, while $Cd(NH_2SO_3)_2$ exhibits a 3D framework made up of *cis*-$[CdO_4(NH_2)_2]$ octahedra and $[NH_2SO_3]$ tetrahedra. For the first time, nitrogen-containing $[CdO_4N_2]$ octahedra are observed in the metal sulfamates. The unique arrangement is discussed using the hard-and-soft acids and bases theory and compared with other existing $[MO_6]$ (M = Na, Mg) octahedra in sulfamates. $Cd(NH_2SO_3)_2$ has a phase-matchable SHG response of approximately 0.15 × KDP. Interestingly, reversible phase transitions induced by temperature and humidity are observed between these two compounds. The insertion of water molecules suggests the flexibility of the metal sulfamate frameworks and features a switchable SHG ability of the two cadmium sulfamates.

Poster Presentation : **INOR.P-54**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis, characterization, and theoretical investigations of a rare-earth selenite with well-balanced nonlinear optical functionality

Zhiyong Bai, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

High-performance ultraviolet (UV) nonlinear optical (NLO) materials were urgently needed, but their development remains a significant challenge owing to the contradictory behavior among three core indicators: second-harmonic generation (SHG) efficiency, band gap (absorption edge), and birefringence. Currently, the search for UV NLO materials is mainly focused on the borates and phosphates. In this work, the exploration of high-performance UV NLO materials was extended to the selenite system, resulting in the synthesis and characterization of a targeted compound, the rare-earth selenite, $Sc(HSeO_3)_3$. The title compound crystallizes in the polar noncentrosymmetric space group, *Cc*and its crystal structure is composed of interlinked ScO_6 octahedra and $HSeO_3$ groups. Remarkably, the reported material exhibits well-balanced UV-NLO functionality, including the shortest absorption edge (~214 nm) among NLO-active selenites, a wide band gap (5.28 eV), a large phase-matchable SHG response (5 × KDP), and sufficiently large birefringence (cal. 0.105 @1064 nm). Detailed DFT calculations have been performed to elucidate the structure-property relationships of the material.

Poster Presentation : **INOR.P-55**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of hybrid Nano Flake-like VSe2@MWCNT as a Binder-Free Electrode for Sodium-Ion Batteries

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Nowadays, the importance of energy storage is being emphasized. Research on sodium-ion batteries (SIBs) is being conducted thanks to resource-abundant and price-effective advantages compared to lithium-ion batteries (LIBs). Generally, it is inappropriate to apply graphite, which is commercially used for anode materials for LIBs, to SIBs because of its low capacity. We synthesized the materials applicable to anode electrodes for SIBs. Nano flake-like vanadium diselenide (VSe2) synthesized by a colloidal method and hybridized with multi-walled carbon nanotubes (MWCNT). VSe2 is suitable for use as anode materials for SIBs as follows: VSe2 (1) has large interlayer spacing (6.11 Å) and (2) exhibits high theoretical capacity showing the conversion reaction. Using MWCNT, an electrode was fabricated without binder and substrate through a vacuum filter. The electrochemical tests were conducted using a half-coin cell in a voltage range of 0.01 to 2.7 V versus Na/Na+. The VSe2@MWCNT electrode exhibits a good discharge capacity of 469.1 mAhg-1 and coulombic efficiency of 99.7 % at a current density of 0.01 Ag-1 after 200 cycles. The hybrid anode also shows high-rate capabilities in the current range from 0.05 to 2 Ag-1. This work showed several advantages of our materials as anodes for SIBs.

Poster Presentation : **INOR.P-56**

Inorganic Chemistry

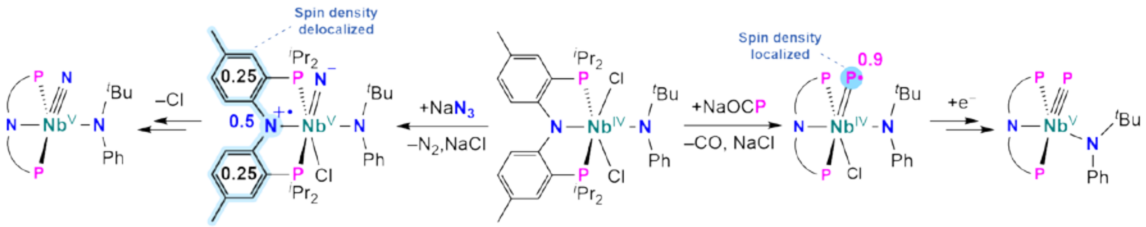
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Understanding the Electronic Structure of Niobium Nitride and Phosphide

Hoyoung Im, **Seongyeon Kwon**, **Mu-Hyun Baik***

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Metal nitride and phosphide complexes are important reagents for organic compound synthesis containing nitrogen and phosphorus. Recently, we successfully synthesized and identified niobium-nitride and niobium-phosphide complexes stabilized by the PNP-type pincer ligand (Bis(2-(diisopropylphosphaneyl)-4-methylphenyl)amide). We conducted density functional theory calculations to investigate the reaction mechanism involved in the formation of these compounds and identified different roles of the pincer ligand during the reaction. Specifically, the redox non-innocent behavior of the pincer ligand was only observed in the formation of the niobium-nitride compound, supporting the formation of the strong Nb(V)≡N triple bond. In contrast, the counterpart for niobium-phosphide formation featured a weaker Nb=P double bond, rendering spin density localized on the phosphorus atom. We concluded that this redox non-innocent behavior arises from the relative energy levels of the frontier orbitals between the pincer ligand and the Nb–X (X = N, P) bonds. We are currently planning to design a new type of pincer ligand with precise control of frontier orbitals to induce redox non-innocent behavior and promote the reactivity of Nb complexes.



131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **INOR.P-57**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrochemical analysis and application of perylene diimide substituted with an amino acid as an organic cathode for lithium-ion batteries

Honggyu Seong, Chan Woong Na[1], Yoon Myung[1], Jaewon Choi*

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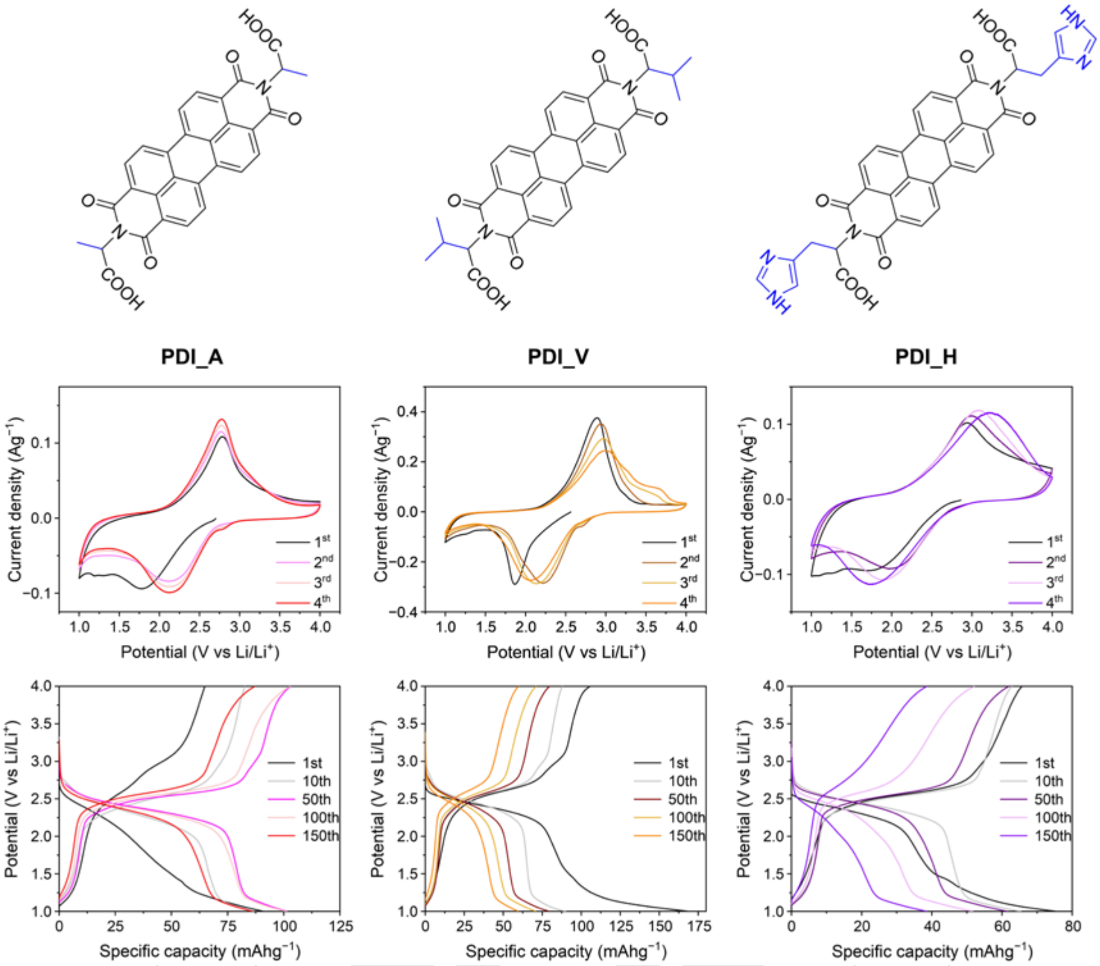
[1]*Korea Institute of Industrial Technology, Korea*

Organic-based materials are considered alternatives with benefits such as abundant resources, flexibility, and green engineering. In this work, we synthesized three derivatives of perylene substituted with L-amino acids (PDI_AAs) and labeled them as PDI_A (L-alanine), PDI_V (L-valine), and PDI_H (L-histidine), respectively. Also, the cyclic voltammogram of PDI_AAs showed the redox activity and the reversibility of the lithiation-delithiation process. Furthermore, PDI_A showed the best performances among the PDI_AAs cathodes with a capacity of 86 mAh g^{-1} (95 % retention) over 150 cycles. It also revealed outstanding long-term cycling performances with a capacity of 47 mAh g^{-1} (98 % retention) over 5,000 cycles. To study the charge-discharge mechanism of PDI_A cathodes, we conducted an ex-situ ATR FT-IR analysis of electrodes of different charged states, which revealed the structure of charged PDI_A as lithium enolate coordinated with a carboxylic acid. Thus, these results will contribute to the development of next-generation organic cathodes.


HOOC
COOH
HN
NH
PDI_A
PDI_V
PDI_H
Current density (Ag^{-1})
Potential (V vs Li/Li^{+})
1st
2nd
3rd
4th
Potential (V vs Li/Li^{+})
Specific capacity (mAhg^{-1})
1st
10th
50th
100th
150th

Poster Presentation : **INOR.P-58**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Improving CO_2 Adsorption Capacity of Nitrogen-Enriched Polytriazine by Incorporating Transition Metal Atoms: A DFT Study

Hieu minh Ngo, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Nitrogen-enriched polytriazine (NPT), a carbon nitride-based material, has received significant attention for its potential application in CO_2 storage. To enhance its CO_2 uptake capacity, it is imperative to comprehend the interaction mechanism between CO_2 molecules and NPT. In this study, we propose a novel approach to improve the CO_2 adsorption ability of NPT by incorporating Sn, Co, and Ni metal atoms into the polytriazine network. Using DFT calculations, we investigated the CO_2 adsorption mechanism of the polytriazine frameworks by examining the interactions between CO_2 and the different interaction sites of NPT. By optimizing the geometry of the pure and metal-containing NPT frameworks, we determined the binding energy of metal atoms in the NPT framework, the adsorption energy of CO_2 molecules, and the charge transfer between CO_2 molecules and the corresponding adsorption systems. Our findings demonstrate that introducing transition metal atoms into the cavities of NPT can significantly increase its CO_2 adsorption capacity.

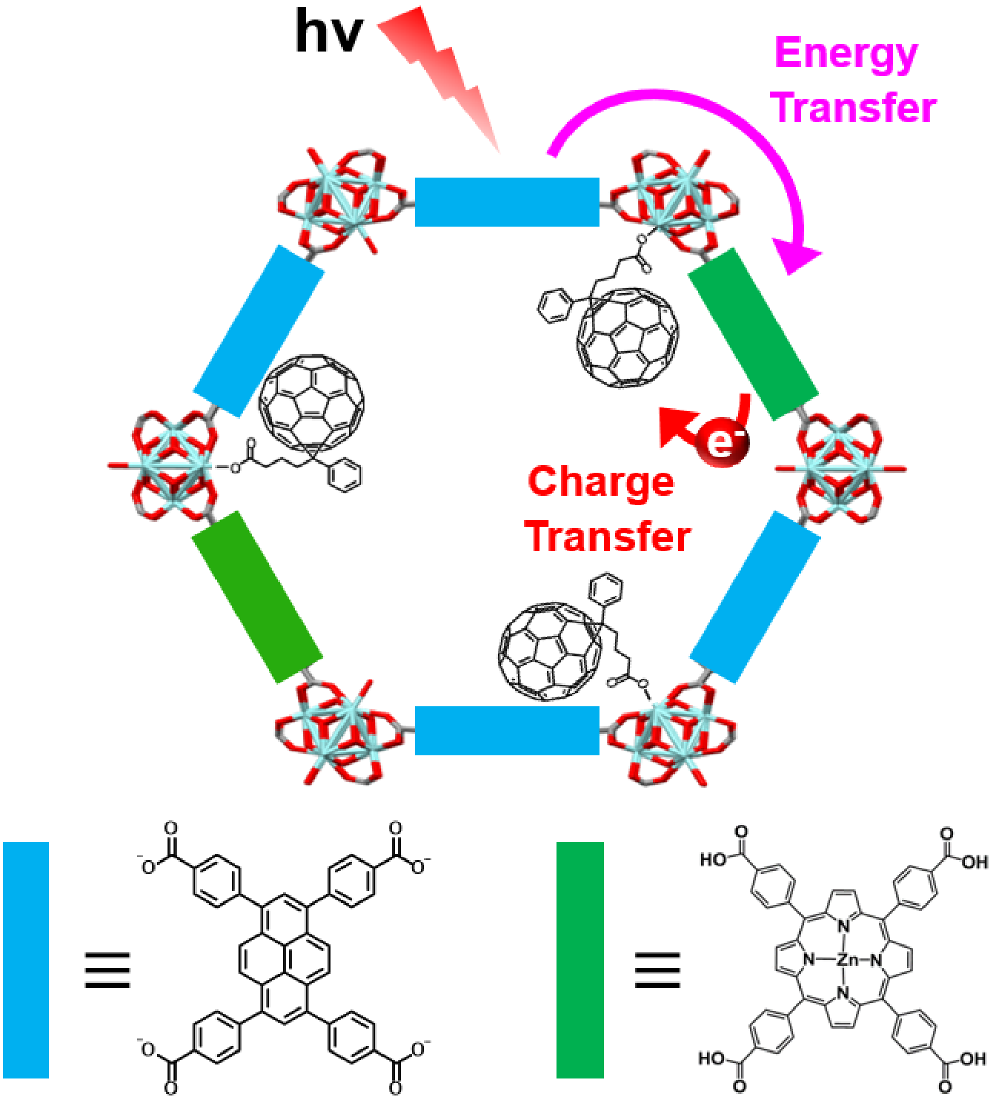
Poster Presentation : **INOR.P-59**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Enhancement of Photocatalytic performance via C_{60}-incorporated Nano Mixed Ligand MOFs (nMLM)

Woo Seong Jo, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Photocatalytic reaction using energy from the infinite sunlight is being used for environmentally friendly CO_2 reduction, and decomposition of organic pollutants, and hydrogen production. Light is irradiated to the photosensitizer to generate electron-hole pair, and the photosensitizer in an excited state transfers energy to triplet oxygen to generate reactive oxygen species (ROS). To produce these ROS effectively, electron-hole recombination must be minimized in the photocatalyst. Recently, we developed a nanosize mixed-ligand MOF (nMLM) by reacting a Zr metal cluster with a mixture of Pyrene and Porphyrin building units which suppressed electron-hole recombination by ligand-to-ligand Energy Transfer. Herein, we further constructed a three-stage of EnT (Energy transfer), CT (Charge Transfer) system from C_{60} electron acceptor by SALI (Solvent-Assisted Ligand Incorporation) of C_{60} to nMLM. This system has sequential Energy and Charge transfer order and prevents electron-hole recombination so that it shows high efficiency of ROS generation. The C_{60}@nMLM Triad system showed excellent photocatalytic performance at ROS generation.


hν
Energy Transfer
e⁻
Charge Transfer
≡
≡
Zn
N
HO
OH
O

Poster Presentation : **INOR.P-60**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effective photodynamic therapy for acute vascular occlusion using an iron-nitrosyl complex

Jisu Choe, Mu-Hyun Baik[1,*], Jaeheung Cho[2,*]

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

Retinal vascular occlusion is a common cause of visual impairment. Although several approaches, including vasodilators, have been explored to treat retinal vascular occlusion, there is no proper method to treat this obstruction today. We report a strategy that aims to pierce clogged blood vessels with a spatiotemporally controllable nitric oxide transporter, $[Fe(TBDAP)(NO)(H_2O)]^{2+}$ (TBDAP = *N,N'*-di-*tert*-butyl-2,11-diaza[3.3](2,6)pyridinophane), which was synthesized and precisely characterized by various physicochemical methods, including X-ray crystallography. In the animal model, normal retinal blood vessels were confirmed to be dilated by the photo-responsive iron–nitrosyl complex. Furthermore, occluded retinal blood vessels were effectively reperfused after the immediate delivery of nitric oxide using light in animal disease models. These studies suggest an unprecedentedly selective and controllable treatment option for acute vascular occlusive diseases, including cardiovascular and cerebrovascular diseases.

Poster Presentation : **INOR.P-61**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of zwitterionic polymer-modified metal-organic frameworks as a solid-state electrolyte

Yeji Lee, Hyerin Woo, Sarah Sunah Park[*]

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

Solid-state electrolytes (SSEs) have been attracting a lot of attention as a promising solution for safe lithium metal batteries. However, solid-state polymer electrolytes, which are representative SSE materials, suffer from low and random free volume, and therefore have limitations in confining plasticizers or providing regular ion-pair dissociation sites. To address this issue, this study proposes a synergistic composite with high ionic conductivity, achieved by threading polyelectrolytes into the pores of a metal–organic framework (MOF) at a molecular scale. Specifically, a zwitterionic polymer with a high dipole moment backbone is confined into the MOF via in situ polymerization of encapsulated monomers. Upon complexation with lithium salts, this zwitterionic polymer-modified MOF exhibits high ionic conductivity of 8.84×10^{-4} S cm^{-1} at 25 °C and wide electrochemical stability ranging from 2.3–5.0 V vs. Li^+/Li. Our study investigates the ion pair dissociation behavior of zwitterionic polymers in MOF pores and proposes a novel approach to enhancing the performance of solid electrolytes based on the synergetic effect of MOFs and polyelectrolytes.

Poster Presentation : **INOR.P-62**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Enhancing Charge Trapping and Water Reduction through Pt-CdSe Hybrid Nanorod Photocatalysts with Controlling Cocatalyst Morphology

Bumjin Park, Hyunjoon Song[*]

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

In metal-semiconductor hybrid structures, the morphology and surface nature of metal cocatalysts are expected to be primary elements in approaching ideal photocatalytic systems. Herein, we generated three distinct morphologies of Pt cocatalysts, round, cubic, and rough, in Pt-tipped CdSe nanorods and employed them as hydrogen evolution photocatalysts. By visible light irradiation, hydrogen evolution activity was the maximum at the rough tips, followed by the round and cubic tips. Kinetic investigations with transient absorption spectroscopy informed that the cubic tips lowered carrier dynamics and water reduction rate due to their defectless surface facets. On the other hand, the rough tips showed similar carrier dynamics but a two times faster surface reaction rate than the round tips, resulting in a considerable enhancement of hydrogen evolution. This result indicates that the rational design of the metal cocatalysts is as significant as the main semiconductor bodies to maximize photocatalytic activities.

Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Seeded Living Metallosupramolecular Polymerization by Eu(III) complex

Seol A Lim, Sung Ho Jung[1,*], Jong Hwa Jung[1,*]

Department of Chemistry, GYEONGSANG NATIONAL UNIVERSITY, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

We investigated the seeded living supramolecular polymerization by Eu(III) complex as monomeric species. The seeded living supramolecular polymerization was synthesized using Eu(III) complex. After supramolecular polymerization of Eu(III) complex with terpyridine ligand, The seed ($Eu\text{-}1_{seed}$) of supramolecular polymer based on Eu(III) complex was prepared by ultrasonication at 10 ^{o}C. SEM images showed 200-250 nm of lengths and a narrow polydispersity (PDI = 1.05). After multicycles by seeded living supramolecular polymerization, the lengths of polymers increased without PDI. These results indicate that the living supramolecular polymerization occurred at active termini of seed. The formation of supramolecular polymers was characterized using UV/Vis spectroscopy, fluorescence spectroscopy, scanning electron microscopy (SEM), and dynamic light scattering method (DLS). This study is expected to provide new knowledge on supramolecular polymerization systems involving metal coordination complexes such as metal-metal interactions, metal coordination, fluorescence of metal elements, and coordination geometry changes.

Poster Presentation : **INOR.P-64**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Influence of Ag(I)-coordinated supramolecular architectures by conformation isomers in alkyl chains

Hyeon Min Han, Jong Hwa Jung*, Sung Ho Jung*

Department of Chemistry, Gyeongsang National University, Korea

We report Ag(I)-coordinated supramolecular architectures of a terpyridine-based ligand bearing an alanine moiety and *trans*- or *cis*-double bond in the alkyl chain in the presence of $AgNO_3$ (0.5 and 1.0 equiv.) in H_2O and dimethyl sulfoxide (DMSO) (1:4 v/v). In the presence of $AgNO_3$, *trans*-L exhibited a helical ribbon structure while *cis*-L exhibited a linear ribbon structure. Furthermore, self-assembled *trans*-L exhibited a strong circular dichroism (CD) signal helicity. In contrast, self-assembled *cis*-L formed in the presence of 0.5 and 1.0 equiv. of $AgNO_3$ showed a weak CD signal, indicating that the *cis*-L molecules did not form a helical arrangement in the supramolecular architecture.

Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Two-dimensional $Cu_{2-x}S/CdS$ heterostructured nanoplates via a cation exchange reaction for photocatalytic hydrogen generation under visible light-irradiation

Kodong Bang, Bumjin Park, Hyunjoon Song*

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

Solar-to-fuel conversion using semiconductor materials has been studied for decades as a promising solution for clean and sustainable energy. Among the various reactions, the photocatalytic hydrogen evolution reaction is particularly valuable for clean and renewable energy sources. To enhance photocatalytic efficiencies, heterostructured photocatalysts which are combined with more than two materials are necessary to prohibit charge recombination and increase charge separation. Herein, we report visible light active two-dimensional $Cu_{2-x}S/CdS$ heterostructured nanoplate via a cation exchange reaction using hexagonal $Cu_{2-x}S$ nanoplate as a template. By varying the Cd exchange ratio, we measured the photocatalytic reactivity and focused on the optical properties. For 70% Cd/Cu ratio showed the optimal photocatalytic activity and exhibited a higher hydrogen evolution rate than similar compositions such as the $Cu_{2-x}S/CdS$ one-dimensional nanorod system under visible light irradiation. This work demonstrates the correlation between the Cd^{2+} exchange ratio and charge separation, and a rational design of semiconductor-semiconductor heterojunction on two-dimensional nanostructures for photocatalytic activity.

Poster Presentation : **INOR.P-66**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ultraporous germanium based porous aromatic frameworks for hydrogen storage

Yong Hoon Lee, Sumin Yu[1], Su Min Lee, Sookyung Park, Chang Seop Hong[*]

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

To reduce the environmental impact and the use of fossil fuels, hydrogen, which has a high energy density, is in the spotlight as clean energy solutions. However, current hydrogen storage technologies require exceptionally high pressure or cryogenic temperature, which causes additional loss of energy. Therefore, porous aromatic frameworks (PAFs) are promising adsorbent materials to store hydrogen. PAFs are synthesized by yamamoto coupling, which reaction make highly connected frameworks. the robust covalent C-C bond leads to exceptionally high thermal and chemical stability. Herein, we present germanium-based PAF exhibiting high porosity, robust stability, and outstanding hydrogen storage performance. The textural properties of germanium-based PAF were characterized by N_2 isotherm, FT-IR spectroscopy, thermogravimetric analysis, PXRD measurements and the hydrogen storage property was confirmed through high-pressure hydrogen isotherm. Detailed synthesis, and properties will be presented in poster.

Poster Presentation : **INOR.P-67**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Supramolecular architectures based on binuclear Pt(II) complexes consisting different ligands and circular and helical fiber structures

Minhye Kim, Sung Ho Jung[1,*], Jong Hwa Jung[*]

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

Recently, supramolecular architectures such as helical fiber, tubular, and nanotoroid (nanoring) have attracted significant interest over the past few decades because of their special physical properties. In this study, we synthesized bis[terpyridine-based Pt(II)] complexes with different terminal ligands such as Cl^-, phenyl acetylene, or pyridine units. Interestingly, the binuclear terpyridine-based Pt(II) complex (Ch-1), consisting of Cl^- as one ligand at both ends, forms a circular supramolecular architecture through a net structure as a thermodynamic product via multiple steps. In contrast, the Pt(II) complex (Ph-1) with phenylacetylene groups exhibited a helical fiber structure. The supramolecular architectures were generated by Pt$\cdots$Pt, $\pi-\pi$, and intermolecular hydrogen-bonding interactions. In the presence of pyridine, two Cl^- coordinated to Pt(II) in Ch-1 were converted to pyridine groups to generate a Pt(II) complex (Py-1) with pyridine groups by a ligand exchange reaction, which spontaneously afforded circular to helical fiber structures. The supramolecular architectures were generated by a cooperative pathway involving a nucleation-elongation mechanism. The helical supramolecular polymerization of Py-1 was kinetically controlled by the concentration of pyridine and followed an on-pathway

Poster Presentation : **INOR.P-68**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Multielectron Transfer Photocatalysis of Dinuclear Ir(III)–Re(I) complexes with quaterpyridine bridging ligand: Accumulation of Charges on π-conjugated Linker and Intramolecular Electron Transfer to Re(I) Catalyst

Daehan Lee, Min Su Choe, Min-jong Bong, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Four new sterically-distorted quarter pyridyl (qpy) ligand-bridged Ir(III)-Re(I) heterometallic complexes (Ir-qpy$_{mm}$-Re, Ir-qpy$_{mp}$-Re, Ir-qpy$_{pm}$-Re, and Ir-qpy$_{pp}$-Re) were prepared, along with the fully π-conjugated Ir(III)-Re(I) complexes (π linker = 2,2′-bipyrimidine (bpm), Ir-bpm-Re; π linker = 2,5-di(pyridin-2-yl)pyrazine (dpp), Ir-dpp-Re) to elucidate the electron mediating and accumulative charge separation properties of the bridging π-linker in a bimetallic system. From the photophysical and electrochemical studies, it was found that the qpy bridging ligand (BL), in which the two planar Ir/Re-metalated bipyridine (bpy) ligands were connected but slightly canted relative to each other, linking the heteroleptic Ir(III) photosensitizer, $[(^{piq}C\^{}N)_2Ir^{III}(bpy)]^+$, and catalytic Re(I) complex, $(bpy)Re^{I}(CO)_3Cl$, minimized the energy lowering of the qpy BL, which hampers the forward photoinduced electron transfer (PET) process from $[(^{piq}C\^{}N)_2Ir^{III}(N\^{}N)]^+$ to $(N\^{}N)Re^{I}(CO)_3Cl$ (E_{red1} = -(0.85–0.93) V and E_{red2} = -(1.15–1.30) V vs SCE). Based on a series of anion absorption studies and spectroelectrochemical (SEC) analyses, all Ir(III)-BL-Re(I) bimetallic complexes were found to exist as di-anionic form (Ir(III)-$[BL]^{2-}$-Re(I)) after fast reductive-quenching process in the presence of excess electron donor. In the photolysis experiment, the four Ir-qpy-Re complexes displayed the reasonable photochemical CO_2-to-CO conversion activities (TON of 366–588 for 19 h).

Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photoreactive One-Dimensional Zn(II) Metal-Organic Frameworks by Dicarboxylic Acid with Different Coordination Vectors by Oxygen and Sulfur Atoms

Jaewook An, Jihye Oh, Heekyoung Choi, In-Hyeok Park*

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

Photoreactive one-dimensional (1D) Zn(II) metal-organic frameworks (MOFs, **1** and **2**) using two dicarboxylic acids with different coordination vectors. The pale yellow block-shaped single crystals (**1**) were synthesized by solvothermal reaction of the mixture of Zn(II), 4-stylylpyridine (spy), and 2,5-thiopendicarboxylic acid (H_2tdc). Single crystal X-ray analysis reveals that **1** is composed of [Zn(spy)$_2$(tdc)(H_2O)]·DMA with space group *Pna*2$_1$. The S atoms of tdc ligands were alternately aligned in different directions to form a 1D chain backbone [Zn(tdc)]. On the other hand, [Zn(spy)$_2$(fdc)(H_2O)] (**2**), which has an O atom instead of a sulfur atom as a carboxylic acid, was synthesized as a mixture of Zn(II), spy, and 2,5-furandicarboxylic acid (H_2fdc). When tdc was replaced with fdc, a yellow block-shaped single crystal with a *P*-1 space group was obtained, and the O atoms of fdcs were aligned to face the same direction to form a 1D linear structure. The repeating unit in **1** and **2** are same. They are consisting of octahedrally coordinated Zn(II) ion by four oxygen atoms and two nitrogen atoms from spy ligands and H_2O, respectively in both single crystals **1** and **2**, the double bonds of spy ligands are parallelly aligned and the distance are suitable for photo-cycloaddition reaction in Schmidt's criteria.[1] The photoreactivity of **1** and **2** were also confirmed by ^{1}H nuclear magnetic resonance analysis. The 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-70**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Swellable Porous Organic Polymer for Volatile Organic Compounds Adsorption

Su Min Lee, Sookyung Park, Sumin Yu[1], Yong Hoon Lee, Chang Seop Hong[*]

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

Porous organic polymers (POPs) have been attracted due to their various structures through the combination of different monomers and linkers. In particular, some POPs exhibit structural extensibility that swells in solvents owing to their flexible linkers. The swelling behavior of POPs increases C-H…π interaction between POP networks and adsorbates, allowing their applications for volatile organic compounds (VOCs) adsorption. Herein, we synthesized more than 30 flexible POPs and screened out 3 candidates which show high structural extensibility. Enhanced structural flexibility produces distinctive host-guest interaction, adsorbing xylenes with high adsorption amounts. Moreover, their high chemical stability and facile synthesis made them promising adsorbent candidates for other VOCs. Detailed synthesis and characterization will be presented in the poster.

Poster Presentation : **INOR.P-71**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Bead fabrication of polymer-supported MOF for indoor air capture

Sookyung Park, Su Min Lee, Yong Hoon Lee, Sumin Yu[1], Chang Seop Hong*

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

The concentration of the CO_2 needs to be controlled under 1,000 ppm for human health, since high concentration of CO_2 can make people get fatigue and headache. Metal-organic frameworks (MOF) have significantly studied for CO_2 adsorption, and especially, the MOF-74 variants are one of the prominent adsorbents for CO_2 adsorption. However, the powder form of the MOF is not suitable for real industry owing to the difficulty of handling. Herein, we present the bead form of polymer-supported MOF. The bead exhibited exceptional working capacity at 1,000 ppm CO_2. Hence, we successfully fabricated applicable bead form of polymer-supported MOF for effective CO_2 adsorption at 1,000 ppm. Detailed synthetic scheme and characteristics will be presented in the poster.

Poster Presentation : **INOR.P-72**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effect of bridging ligands of MOF on CO_2 capture

Sumin Yu, Su Min Lee[1], Sookyung Park[1], Yong Hoon Lee[1], Chang Seop Hong[1,*]

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

Metal-organic frameworks (MOFs) with high surface area, tunable pore size, and low heat capacity are in the spotlight as CO_2 adsorbents. Among them, Ni_2Cl_2BTDD with hexagonal rod shape features open metal sites, high surface area, and exchangeable bridging ligand. Herein, we replaced the structural bridging Cl with OR (R=H,CH_3,$CH_2(CH_3)$,$CH(CH_3)_2$, $C(CH_3)_3$) to examine the effect of bridging ligand on CO_2 capture. When the bridging ligand was exchanged with the OH, CO_2 uptake increased almost three and six times at low and high pressure, respectively. As the bridging ligand became heavier, CO_2 uptake showed a tendency to decrease. Exceptionally, in the case of $OC(CH_3)_3$ exchanged MOF, it exhibited steep CO_2 adsorption at extremely low pressure, forming many interactions with CO_2. Detailed synthesis and characterization methods will be presented in the poster.

Poster Presentation : **INOR.P-73**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Gas Sorption Study of Metal-Organic Framework Comprising Mixed Metal (Mg/Mn) Ions

Bonseon Eo, Younghu Son[1], Gyungse Park[2], Minyoung Yoon[3,*]

Chemistry, Kyungpook National University, Korea
[1]*Department of Chemistry, Kyungpook National University, Korea*
[2]*Department of Chemistry, Kunsan National University, Korea*
[3]*Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea*

Metal-organic frameworks (MOFs) are a fascinating class of materials with a wide range of potential applications. By mixing different metals and ligands, it is possible to tune their properties to suit specific needs. Recently, MOFs have attracted attention due to their high framework stability and highly selective gas adsorption properties, which makes them promising for gas separation and storage applications. Also, varying the mixing ratio of metals in the MOFs is a useful approach to understand the effect of metal composition on gas adsorption properties. In this study, we demonstrate N2 H2, and CO2 adsorption capabilities with MOFs synthesized by magnesium (Mg) and manganese (Mn) that consisted with formate ions (HCO2−), which has a microporous and diamond network structure denoted as M(HCO2)2 (where M = Mg2+ or Mn2+). In addition, we synthesized the different mixing ratio of the two metal ions to investigate the effect on gas adsorption properties (the mixing ratio is as follows: 1:3, 1:1, and 3:1 of Mg:Mn). Our results demonstrate that the adsorbed amount of N2 and H2 gases varies depending on the mixing ratio of metals. To our knowledge, there have been no previous studies on the adsorption properties of mixed-metal MOFs with varying Mg/Mn ratios. In addition, the grand-canonical Monte Carlo (GC-MC) calculation suggests the sorption property of the MOFs. Therefore, our study showed the adsorption properties of mixed metal MOFs that provide important insights into the effect of metal composition and suggest the potential of these materials for gas separation and storage applications.

Poster Presentation : **INOR.P-74**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Introduction of Carbon Shells on Copper Oxide Nanocrystals Inducing CO2-to-Methane Electroconversion

Jong-Yeong Jung, Hyunjoon Song[*]

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

The electroconversion of CO2 to methane on a large scale is one of the most attractive goals to achieve a carbon-neutral economy. However, methane production with high current density is a general challenge due to the facilitated C–C coupling and hydrogen evolution reaction leading to C2+ products and H2 gas. The role of the oxidation state of the copper species in electrochemical CO2 reduction has been highlighted to regulate the products. In this work, we introduced amorphous carbon shells composed of polyimide bonds on cuprous oxide nanocubes to remain copper in the +1 oxidation states under the reduction potential. As the thickness of the carbon shell increased, methane selectivity dramatically improved and saturated. We optimized the depth of carbon shells with 50 nm and the resulting core/shell structured Cu2O/C displayed improved methane selectivity, reaching Faradaic efficiency of 50.2 ± 3.9% at a methane partial current density of −201 ± 16 mA cm−2 in alkaline electrolytes. Operando X-ray absorption near edge structures (XANES) spectra at the Cu K-edge and in situ Raman spectra confirmed that introduced amorphous shell induced high local pH and stabilize Cu+ species stabilized during CO2RR.

Poster Presentation : **INOR.P-75**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Thermodynamically controlled supramolecular polymers based on Pt complex

Kayeong Go, Sung Ho Jung[1,*], Jong Hwa Jung[*]

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

Chiral self-assembled aggregates are an efficient chiral emission source, potentially applicable and still an active field in research. Thus, terpyridine-based Pt complex (L-Pt) having R- or S-alanine moiety was synthesized. To demonstrate Pt-Pt interaction in different compositions of H_2O and DMSO, emission spectra were observed by photoluminescence (PL) spectroscopy. In H_2O and DMSO (4:1 v/v), PL spectrum of L-Pt was obtained at ca. 700 nm, corresponding to MMLCT. With increase of DMSO, emission shifted to short wavelength, which was attributed to weak MMLCT interaction. Supramolecular polymer showed the fiber structures with right-handed helicity. Furthermore, thermodynamic study was performed by UV-Vis spectroscopy

Poster Presentation : **INOR.P-76**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Morphological Changes of Supramolecular Copolymers Made of Pt Complexes

Sehee Kim, Sung Ho Jung[1,*], Jong Hwa Jung[*]

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

Random copolymerization is an effective approach to synthesize polymers with the properties of harmonizing different monomers. Ensuring that monomers with distinct molecular structures and properties reach random copolymers is a difficult problem because of the enthalpic advantage of self-recognition (self-sorting). A study was conducted on the subject of the random supramolecular copolymerization of two thermodynamically controlled monomers. A Pt complex ligand having a terpyridine and a phenylacetylene groups was synthesized by several steps. The MMLCT interaction in supramolecular polymer was confirmed by PL spectroscopy. In addition, supramolecular polymer showed the right- and the left-handed helicities by SEM observation.

Poster Presentation : **INOR.P-77**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

P3HT Polymer-Sensitized TiO_2 Catalysts for Sustainable Photochemical Carbon Dioxide Reduction

Min Su Choe, Daehan Lee, Min-jong Bong[1], Sang Ook Kang, Ho-Jin Son[2,*]

Department of Advanced Materials Chemistry, Korea University, Korea
[1]*Korea University, Korea*
[2]*Department of Advanced Materials Chemistry, Korea University, Sejong, Korea*

In this study, poly(3-hexylthiophene-2,5-diyl) (P3HT), was physically adsorbed onto n-type TiO_2 nanoparticles functionalized with a molecular CO_2 reduction catalyst, (4,4-Y_2-bpy)ReI$(CO)_3$Cl (ReP, Y = $CH_2PO(OH)_2$), to generate a new type of P3HT-heterogenized hybrid system (P3HT/TiO_2/ReP). We found that the heterogenization of P3HT onto TiO_2 resulted in a steady electron supply toward the co-adsorbed Re(I) catalyst, attaining durable catalytic activity with a turnover number (TON) of ~5,300 over an extended time period of 655 h over five consecutive photoreactions, without deformation of the adsorbed P3HT polymer. The long-period structural stability of TiO_2-adsorbed P3HT was verified based on a comparative analysis of its photophysical properties before and after 655 h of photolysis.

Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Secondary Sphere Effect on Monobipyridyl Mn(I) Catalysts in Photochemical CO_2 Reduction: Efficient Product Selectivity Modulation by alcohol and alkyloxy Tethering ligands

Min-jong Bong, Daehan Lee[1], Min Su Choe[1], Sang Ook Kang[1], Ho-Jin Son[1,*]

Korea University, Korea

[1]*Department of Advanced Materials Chemistry, Korea University, Korea*

While the incorporation of pendant Brønsted acid/Lewis base sites in the secondary coordination sphere is a promising and effective strategy to increase the catalytic performance and product selectivity in organometallic catalysis for CO_2 reduction, the control of product selectivity still faces a great challenge. Through the formation of pendant alcohol groups in bipyridine, we want to increase product selectivity by creating a Brønsted acid tethering ligand that directly provides proton to metal and creating a Lewis base site through methoxy and ethoxy groups. In the series of photolysis experiments, compared to nontethered case, the asymmetric attachment of tethering ligand to the bpy ligand led to less efficient but more selective formate production with inactivation of CO_2-to-CO conversion route during photoreaction. Also, the incorporation of bulky tethering ligands prevented Mn-Mn dimerization.

Poster Presentation : **INOR.P-79**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Unpacking the Impact of Increasing Tethering Ligands on Efficiency and Selectivity in Organometallic Catalysts for CO_2 Reduction

Min-jong Bong, Daehan Lee[1], Min Su Choe[1], Sang Ook Kang[1], Ho-Jin Son[1,*]

Korea University, Korea
[1]*Department of Advanced Materials Chemistry, Korea University, Korea*

Increasing catalyst performance and controlling product selectivity in organometallic catalysts for CO_2reduction are major challenges. When pendant Brønsted acid/Lewis bases are combined with secondary coordination sphere, the proton of the tethering ligand can directly supply the proton to the metal, and the metal hydride intermediate can be stabilized by hydrogen bonding between the tether ligand and the metal hydride to increase catalyst efficiency. On the other hand, the number of tethering ligands directly related to the efficiency of CO_2-to-formate conversion: as the number of tethering ligands increased, the structure of the catalyst was bulky, further preventing Mn-Mn dimerization and increasing the product selectivity toward CO_2-to-formate.

Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Converging Hydrogen Bonds Control the Chemistry at Distant Metal Center

Heechan Kim, Kyunghwan Min[1], Dongwhan Lee[2,*]

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

Noncovalent interactions are important players in biological structure and function. Structural modifications of secondary coordination sphere regulate the reactivity of metalloenzymes, even when they share structurally similar primary coordination sphere. One of the key questions is to what extent peripheral hydrogen bonds (HBs) impact the chemistry at distant metal centers. To address this question in a quantitative manner, we built redox-active iron complexes with systematically varied HBs in the secondary coordination sphere. A series of para-functionalized pyridyl pendants was installed around a common tridentate 2,6-bis(benzimidazolyl)pyridine core, establishing a converging network of intramolecular HB, the strength of which was modulated by the electron-donating ability of the pyridine substituents. Despite having an essentially identical primary coordination sphere, the redox chemistry of the resulting iron(II) bis(chelate) complexes is profoundly impacted by the strength of the remotely located HBs. This presentation highlights the primary functional role of (what has often been marginalized as) the secondary coordination sphere.

Poster Presentation : **INOR.P-81**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Study on the Aldehyde Deformylation Reaction Mechanism Catalyzed by a Co(III)-Peroxo Species Using Density Functional Theory

Youngseob Lee, Kyung-Bin Cho[1,*], Hugo Vazquez-Lima[2,*]

Chemistry, Jeonbuk National University, Korea
[1]*Department of Chemistry, Jeonbuk National University, Sweden*
[2]*Chemistry, Meritorious Autonomous University of Puebla, Mexico*

Aldehyde deformylation reaction is one of the important reactions in biology and bioinorganic chemistry. For instance, in the case of Cytochrome P450 aromatase, deformylation reaction is a major process in the production of estrogen, a sex hormone. Many biomimetic studies have studied the aldehyde deformylation reaction mechanism, which is conducted by metal catalyst complexes containing for example iron, manganese, and cobalt as central metals. In this study, we investigate $[Co^{II}(BQCN)(H_2O)(CH_3CN)]^{2+}$ (BQCN = N,N'-dimethyl-N,N'-bis(8-quinolyl)cyclohexane-diamine), a newly synthesized monoclear cobalt(II) compound which reacts with H_2O_2 in acetonitrile in the presence of trimethylamine to produce the Co(III)-peroxo species $[Co^{III}(BQCN)(O_2H)]^{2+}$. The Co(III)-peroxo species perform the deformation reaction of 2-phenylpropionaldehyde to form acetophenone as the final product. The aldehyde deformation reaction mechanism catalyzed by the Co(III)-peroxo species was studied by density functional theory (DFT). Because the possible spin multiplicities of the Co(III)-peroxo species are S=0, S=1, and S=2, the reaction mechanism was calculated for all the three spin multiplicities. As a result of the calculation, the transition states considered as rate determination steps were found to be the C-H activation and C-O bond formation steps at S=2, and the energy was 18.7 kcal/mol and 18.5 kcal/mol compared to the starting point, respectively. So far, about 10 transition states have been calculated for each spin state, and almost all of the mechanism steps have been characterized.

Poster Presentation : **INOR.P-82**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Particle size control of a Cu-based zeolitic imidazolate framework

Jiwon Lee, Yeonjae Kim, Jaheon Kim*

Department of Chemistry, Soongsil University, Korea

A Cu-based zeolitic imidazolate framework Cu-ZIF-rho has a framework of RHO topology in which flattened tetrahedral Cu(II) ions are connected to 2-nitroimidazolate linkers. Cu-ZIF-rho made by solvothermal synthesis was obtained as single crystals of ~10 μm, with a BET surface area of 1322 m^2/g and monolayer capacity of 304 $cm^3/g(P/P_0 = 0.02)$. By adjusting the synthesis method, we obtained Cu-ZIF-rho as a ~0.5 μm crystalline powder in a short time at room temperature and confirmed that it had the same porosity as single-crystal Cu-ZIF-rho. This presentation discusses the synthesis methods of Cu-ZIF-rho and compares the chemical stability and packing efficiency dependent on the particle size.

Poster Presentation : **INOR.P-83**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Cellobiose hydrolysis of covalent organic frameworks functionalized with amino acids

Jeongseon Min, You Jin Oh, Jiwon Lee, Jaheon Kim[*]

Department of Chemistry, Soongsil University, Korea

Cellulase-mimicking catalysts can hydrolyze cellulose into glucose, eventually enabling the regeneration of cellulose into high-value-added organic compounds. We investigated the catalytic activity of covalent organic frameworks (COFs) functionalized with amino acids. After synthesizing a COF backbone by linking tetrakis-(4-phenylboronic acid pinacol ester)methane and 1,4-dibromoaniline through Suzuki-Miyaura coupling, aspartic acid was introduced into the $-NH_2$ group to mimic the active site of cellobiase. Although the conversion of cellobiose to glucose by COF-1-Asp is only 24%, this study shows how to develop a COF catalyst for cellulose hydrolysis. We also propose an alternative synthetic route to achieve amino acid-bound catalytic COFs.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Enhancing gas uptake of a CdS-type metal-organic framework by an exchange of coordinated solvent molecules

Yeonjae Kim, Jeongseon Min, Jaheon Kim[*]

Department of Chemistry, Soongsil University, Korea

CuTNBPDC-1, a doubly-interpenetrated CdS-type metal-organic framework, is synthesized from Cu(II) ions and 2,2’-6,6’-tetranitrobiphenyldicarboxylic acid ($H_2(NO_2)_4BPDC$) via a solvothermal reaction in DMF/MeOH. The DMF molecules bound to the Cu paddle-wheel clusters of CuTNBPDC-1 are firmly enclosed between two frameworks. Due to the interpenetration, the available free volume of CuTNBPDC-1 is only 310 Å^3 with a small BET surface area of 320 m^2/g. With the replacement of DMFs with acetonitrile molecules, the free volume and BET surface area increases to 456 Å^3 and 490 m^2/g, respectively. In addition, CO_2 adsorption at 263 K increases by 47 %, and H_2 at 77 K increases by 31%. CuTNBPDC-1 is stable in water for at least two weeks.

Poster Presentation : **INOR.P-85**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chemical Reconstruction of Bismuth Oxyiodides to Form Sub-carbonate for CO_2 Conversion

Taewaen Lim, Junhyeok Seo*

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

Reconstruction of heterogeneous catalysts by electrochemical conditions is critical for the catalytic performance of CO_2 reduction because the performance should be affected by the surface of catalysts. Thus, the reconstructed species should be thoroughly investigated to study surface chemistry for the improvement of catalysis. Herein, we investigated the chemical reconstruction of bismuth oxyiodides by $KHCO_3$ electrolyte and the catalytic performance for formate production of reconstructed catalysts. The $KHCO_3$ reconstructed orthorhombic and tetragonal bismuth oxyiodides (*t*-BiOI and *o*-Bi_5O_7I) to form $(BiO)_2CO_3$ (BOC-*t* and BOC-*o*) with different morphological and catalytic properties in mild conditions. The BOC-*o* exhibited sharp edge side exposing carbonate species and better performance up to 10 % than BOC-*t* at low overpotential ranges (–0.66 ~ –0.96 V vs. RHE). This is because CO_3^{2-} is active for formate production and BOC-*o* exposed CO_3^{2-} sites, which are contained in the side facet induced by chemical reconstruction. This study provides that the electrolytes can significantly affect the catalysis for CO_2 reduction and CO_3^{2-} sites improve the performance of electrochemical CO_2 conversion to formate.

Poster Presentation : **INOR.P-86**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrocatalytic Hydrogen Evolution Reaction using Molybdenum Oxo Bis(dithiolene) Complexes

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. Unlike earth-abundant transition metals such as Ni, Co, and Fe with square planar structures, 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, Molybdenum-oxo ligand, depending on the acidity of the proton source. Electrocatalytic hydrogen evolution reaction was performed and a reversible shift of onset potential was observed by continuously applying low potential and high potential alternatively. In addition, the effect of cation on lowering the onset potential will be discussed at high pK_a conditions where hydrogen bonding interactions are formed.

Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electronic Effect on Phenoxide Migration at a Nickel(II) Center Supported by a Tridentate Bis(phosphinophenyl)phosphido Ligand

Kunwoo Lee, Yunho Lee[1,*]

Chemistry, Seoul National University, Korea

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

A phosphidenickel(II) alkoxide pincer complex reacts with CO(g) to give a pseudo-tetrahedral nickel(0) monocarbonyl complex possessing a phosphinite moiety. This metal ligand cooperative transformation occurs with a (PPP)Ni scaffold (PPP– = P[2-PiPr2–C6H4]2–). The 2-electron reduction of a nickel(II) species induced by a CO coordination involves group transfer to generate a P–O bond. For better mechanistic understanding, a series of nickel(II) phenolate complexes were prepared. Kinetic experimental data reveal that a phenolate species with an electron withdrawing group reacts faster than those with electron donating groups. The reaction kinetic experiments were conducted in pseudo-first order conditions at room temperature monitored by UV-vis spectroscopy. A pentafluorophenolate nickel(II) complex (2e) reveals instantaneous reactions for forward to give a nickel(0) monocarbonyl species and also for reverse reaction. According to kinetic experiments, the rate determining step would be the formation of a 5-coordinate intermediate 4 with a negative entropy value, and a positive rho value based on the Hammett plot indicates that the electron deficient phenolate leads to the faster CO association. The cationic nickel monocarbonyl intermediate can possess a P—Ni(II), P•–Ni(I) or even P+–Ni(0) character. Another possible reaction is homolysis of a Ni–O bond to give P—Ni(I) or P•–Ni(0), when a phenoxyl radical is liberated. Considering the P–O bond formation, closed-shell nucleophilic and open-shell radical pathways are suggested. A phenolate pathway reveals a lower energy state for 2e relative to other complexes. Therefore, the formation of a P–O bond may occur with the binding of a closed-shell phenolate to the electron deficient P center.

Poster Presentation : **INOR.P-88**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nickel-catalyzed conversion of nitrate (NO3–) and nitrite (NO2–) anion into value-added organic products

Jeewon Chun, Yunho Lee[1,*]

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

The reduction of nitrogen oxides (NOx) is crucial to balance the global nitrogen cycle, as NOx is a serious environmental pollutant generated by human activity. Analogous to the biological denitrification process, a pincer-type nickel scaffold has been previously devised to deoxygenate the NOx to produce dinitrogen (N2). However, the generation of N2 is economically meaningless and further exploration is needed in NOx conversion studies. In this regard, a novel catalysis based on a Ni pincer system supported by a rigidified acriPNP scaffold (acriPNP– = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide) has been introduced, effectively converting Ni–NOx to Ni–NO through deoxygenation with CO(g) in a stepwise manner. The catalyst acts efficiently to transfer the nitroso group from the Ni–NO moiety to alkyl halides, resulting in the formation of nitroso alkanes that tautomerize to form oxime compounds with a turnover number of >200 under mild conditions. While the resulting products of nitrite-deoxygenation were useful, the usage of nitrate anion remains challenging and a detailed reaction mechanism of nitrate deoxygenation need to be evaluated. Therefore, to understand the mechanism involved in the conversion of the nickel-nitrate complex, [(acriPNP)Ni(NO3)] (1) to a nickel-nitro species [(acriPNP)Ni(NO2)] (2), detailed kinetic and theoretical studies have been undertaken. As a consequence, a nickel-carbonyl species, [(acriPNP)Ni(CO)]+ was identified to act as an important intermediate during the deoxygenation of a nitrate anion. Additionally, the nitrate (NO3–) anion has been utilized as the NO-resource for the catalytic NOx conversion to produce value-added oxime compounds from alkyl electrophiles. This innovative NOx conversion and utilization (NCU) technology is an essential step toward achieving a sustainable N-neutral chemical industry.

Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

β-NiOOH Enclosed Ni Nanoplates for Highly Active and Stable Anion Exchange Membrane Water Electrolyzer

Jeonghyeon Kim, Sang-Il Choi[1,*]

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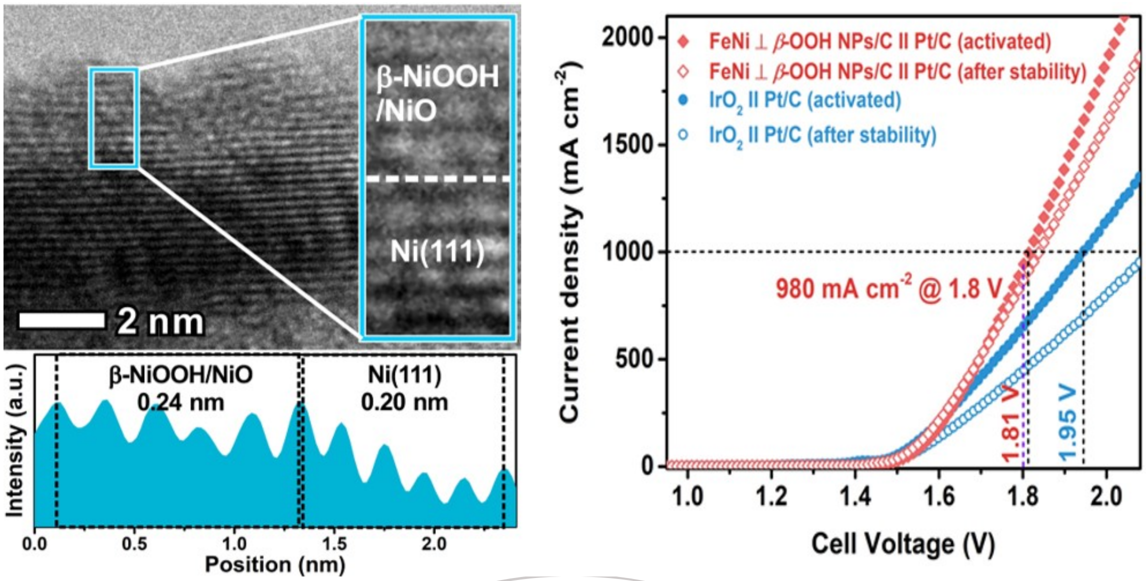
Hydrogen is considered an alternative energy source to replace fossil fuels mitigating carbon emission, and can be produced domestically. High-purity hydrogen production via anion exchange membrane water electrolyzer (AEMWE) recently gained increasing attention due to its potential to achieve low-cost and high-performance water electrolysis. Further to improve the electrolyzer performance, a highly stable and active nanocatalyst is needed for the anodic oxygen evolution reaction (OER), which is the bottleneck of the overall electrolysis process. Ni oxyhydroxides (*β*-NiOOH) on Ni{111} have shown promising activity and stability toward OER in alkaline media. Herein, we report the Fe doped Ni nanoplates (FeNi⊥*β*-OOH NPs) enclosed by *β*-NiOOH with a superior OER stability performance at a constant current density of 10 mA cm^{-2} for record 120 days. Moreover, AEMWE fabricated with FeNi⊥*β*-OOH NPs/C using catalyst coated substrate method shows a current density of 1,000 mA cm^{-2} at 1.81 V with an energetic record efficiency of 76.0%.


β-NiOOH
/NiO
Ni(111)
2 nm
β-NiOOH/NiO
0.24 nm
Ni(111)
0.20 nm
Intensity (a.u.)
0.0
0.5
1.0
1.5
2.0
Position (nm)
FeNi ⊥ β-OOH NPs/C II Pt/C (activated)
FeNi ⊥ β-OOH NPs/C II Pt/C (after stability)
IrO2 II Pt/C (activated)
IrO2 II Pt/C (after stability)
980 mA cm-2 @ 1.8 V
1.81 V
1.95 V
Current density (mA cm-2)
0
500
1000
1500
2000
1.0
1.2
1.4
1.6
1.8
2.0
Cell Voltage (V)

Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

HKUST-1 activation under dry inert gas flow

Ricardo A. Peralta , Nak Cheon Jeong[1,*], Mariana Diaz Ramirez[2]

Departamento de Quı́mica, UAM, Mexico
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[2]*Physics and Chemsitry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Metal-organic frameworks (MOFs) are three-dimensional porous crystalline networks formed of metal clusters connected by organic linkers. Thanks to the wide chemical diversity of these materials, they have been successfully exploited in applications such as gas separation and storage, catalysis, sensing, and drug delivery. One of the key features for these applications is the presence of open metal sites (OMSs) or coordinatively unsaturated sites (CUSs) in MOFs because OMS are usually the strongest binding sites and can lead to more favored interactions with different sorbate molecules. Usually, activation of OMS is achieved by a two-step activation, where first, the synthesis solvent is exchanged for more labile and volatile solvents; then, the sample is thermally activated under a dynamic vacuum. Activation temperatures are commonly between 100 ºC and 180 ºC and activation times generally vary from a couple of hours to up to 24 h. Such harsh conditions or prolonged activation times could provoke distortion or even collapse of the frameworks. Thus, more efficient and faster activation methodologies are desirable. In this work, we present a detailed study of the dissociation of different solvent molecules, from strong coordinating molecules to very weak coordinating ones, under a controlled flow of dry inert gas (N2 or Ar). Preliminary Raman spectroscopy results show that activation under dry inert gas flow lowers the temperature at which water can be dissociated from copper centers in HKUST-1; that is, for water-containing crystals, most of the OMS is activated at 90 ºC without inert gas flow, while activation temperatures drop to 60 or even 40 ºC, depending on if N2 or Ar flow is used respectively. These results are also confirmed by thermogravimetric analysis.

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Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The role of remaining copper cations for additional cation exchange reaction

Suin Jo, Jongsik Park*

Department of Chemistry, Kyonggi University, Korea

Cation exchange reaction in nanocrystals has received considerable attention for its potential to synthesize unconventional nanostructures. In general, the exchange reaction proceeds stoichiometrically based on the oxidation states of cations to maintain the charge balance within the nanocrystal. Copper sulfide has been widely used as a sacrificial template for cation exchange reactions in accordance with the HSAB theory. Herein, we induced the retention of copper cations within the exchanged materials by utilizing an isovalent cation system. We expect that the remnant copper cations could act as active sites for additional cation exchange reactions, thereby enabling the successful synthesis of novel multiphasic materials.

Poster Presentation : **INOR.P-92**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Distortion of anion sublattices in ionic nanocrystals for bending the nanoplates

Minsung Kim, Jongsik Park*

Department of Chemistry, Kyonggi University, Korea

Cation exchange reaction is a commonly used post-modification method in nanocrystal synthesis that has attracted significant attention due to their ability to create a diverse range of heterointerfaces within the nanocrystals. During the cation exchange reaction, a thermodynamically metastable crystal phase forms due to the relatively low mobility of anions compared to cations, thereby preserving the overall morphology of nanostructures. Nevertheless, the anion sublattices may undergo distortion or reconstruction depending on the surface energy of the template material and the thermodynamically stable phase stability of the final product. Herein, we induced the distortion of anion sublattices at the juxtaposed heterointerface through the partial cation exchange reaction. The changes in lattice parameters within the crystal structure can impose surface strain, which can significantly affect the optical and catalytic properties of the resulting products.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and Properties of Hydrogen-Bondable Gold(I) Complexes with Pyrimidine Derivatives

Jiyeong Song, Young-A Lee*

Department of Chemistry, Jeonbuk National University, Korea

Gold chemistry is applied in various fields like light-emitting sensors, catalysts, and drugs. We report the physical characteristics including luminescence and structures of a series of gold(I) complexes with pyrimidine derivative ligands. The cooperative forces of aurophilic and hydrogen bonding have been used in the self-assembly of diphosphine complexes of gold(I) with the thiolate ligands derived from 2-thiobarbituric acid. The complexes have strong NH···O and/or OH···N hydrogen bonding. We planned experiments that our basic gold(I) complexes react with various guests that could have hydrogen bonding. These complexes could be applicated usefully in multiple fields like pharmaceuticals, medical treatment, and body mechanisms as a sensor or switch.

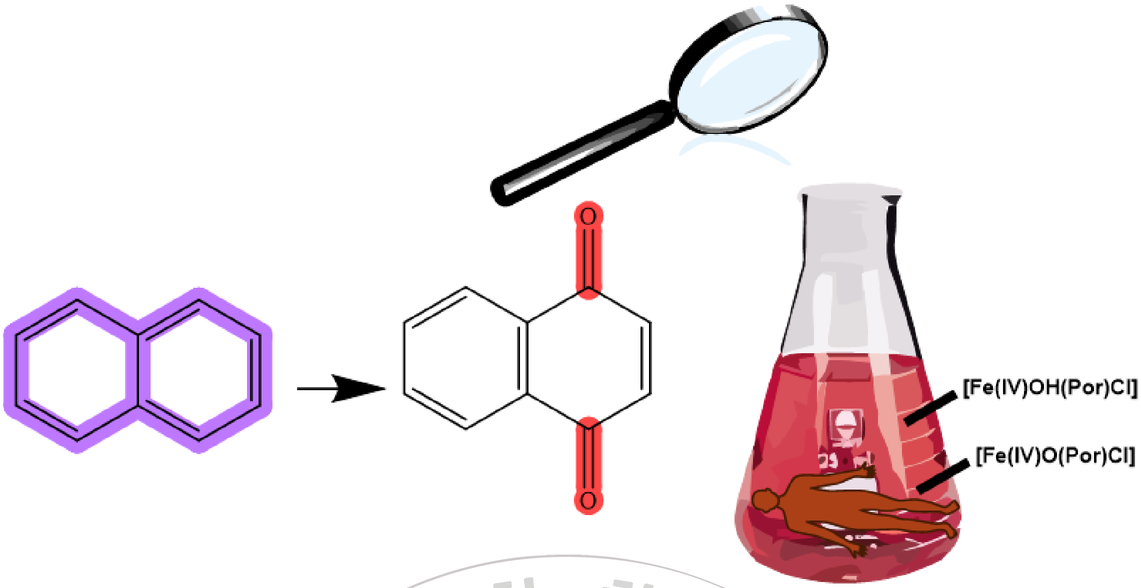
Poster Presentation : **INOR.P-94**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Unraveling the Mysteries of Aromatic Oxidation: A DFT Investigation into [Fe(IV)OHPor(Cl)] Complex's Reaction Mechanism.

Steiny Russelisaac Premakumari, Kyung-Bin Cho[1,*]

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

Developing organometallic catalysts that are green, efficient and stable for the selective direct oxidation of aromatic C-H bonds under mild conditions is a challenging task due to their high stability. Despite this challenge, scientists worldwide are making persistent efforts to improve both catalytic activity and selectivity. We focus on a series of structurally diverse metalloporphyrin compounds, with particular attention given to the high-valent iron and manganese complexes. These complexes serves as key oxidative intermediates in heme and non-heme enzymes, which catalyze essential biochemical processes.[1] This study investigates the direct hydroxylation of aromatic C-H bond using the active catalyst [Fe(IV)OH(Por)Cl]. Through theoretical analysis, the study uncovers the reaction mechanism for the simple aromatic hydroxylation of naphthalene to naphthalene-1,4-diol and its subsequent oxidation to naphthalene-1,4-dione. The investigation reveals that both oxygen atom transfer (OAT) and hydrogen atom transfer (HAT) mechanisms are involved in the studied process.[2] Moreover, a contrasting reactivity pattern is observed during the investigation, where the FeIVOH species is more reactive than the FeIVO species. The study examines the relative oxidative abilities of these two species in a congruent reaction. These findings provide valuable insights into the mechanism of the oxidation reaction and demonstrate the potential of [Fe(IV)OH(Por)Cl] as a catalyst for the efficient production of naphthalene-1,4-dione.[3]Reference(1) Cho, K.; Wu, X.; Lee, Y.; Kwon, Y. H.; Shaik, S.; Nam, W. J. Am. Chem. Soc. 2012, 1–4.(2) Zaragoza, J. P. T.; Cummins, D. C.; Mubarak, M. Q. E.; Siegler, M. A.; De Visser, S. P.; Goldberg, D. P. Inorg. Chem. 2019, 58 (24), 16761–16770.(3) Wang, B.; Wu, P.; Shaik, S. J. Phys. Chem. Lett. 2022, 13 (13), 2871–2877.


O
O
[Fe(IV)OH(Por)Cl]
[Fe(IV)O(Por)Cl]

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Poster Presentation : **INOR.P-95**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Stable Monovalent Copper Iodide Complexes with Bisquinoline Ligands

Eun Su Chae, Hong In Lee[1,*]

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[1]Department of Chemistry, Kyungpook National University, Korea

Copper(I) halide complexes often show photoluminescent properties which are potential for light-emitting devices (LED) or solar cells. Among those Cu(I) iodide complexes with various structures have been reported for such applications. However, successful development of Cu(I) complexes are often hampered by the unstable characteristics of Cu(I) state in aerobic condition. Quinoline type ligands have unique chromophores due to its dicyclic structures. In this study, we have applied two new bis-quinoline ligands to synthesize Cu(I) iodide complexes. The complexes were stable in the air. And one of the complexes, Cu(I)(EbQMA)(I), was found to be 1-D coordination polymer with Cu2I2 cores which is important for the optical properties. In this poster, we discuss the synthesis, structure, powder and solution properties.

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Poster Presentation : **INOR.P-96**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Cellular Senescence of Skin Fibroblasts Cells on Silica Nanobeads Surfaces

Ye Rin Choi, Jin Seok Lee[1,*]

Department of chemistry, Hanyang University, Korea
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Accordingly, We studies to confirm the cause of cellular senescence and to overcome it are being progress. Cellular senescence stressors include oncogenes, replicative stress, reactive oxygen stress (ROS), mitochondrial dysfunction, irradiation, and chemotherapeutic drugs. Here, we induced a chemical stress to Skin Fibroblasts to obtain aging cells. Cell aging was induced through Etoposide (Eto) using WS1 cells, which are Human Skin Fibroblasts. In addition, aging was controlled on the silica nanobead surface, a nanoscale topography. The β-galactosidase expressed during aging was confirmed through X-gal staining, and cell viability was confirmed through MTT assay. In addition, cell migration, speed and Western blot was performed to quantitatively analyze the difference according to cell senescence. These systems will be widely used in cellular aging biotechnology in the future.

Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Monitoring the movement of cells on a substrate patterned with ND

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In this study, we report the successful creation of a substrate with aligned nanodiamonds (ND) using atomic force microscopy (AFM) lithography. The engineered NDs possess an NV(nitrogen vacancy) center that enables photoluminescence (PL) measurements. By utilizing these NV centers, we were able to measure the PL of the NDs. The ND-aligned substrate was used to investigate the behavior of cells, including cell movement and adsorption, by placing them on the substrate. The results of this study demonstrate the potential of using NDs as a tool for studying cell behavior, which could lead to the development of new bio-compatible devices for biomedical applications.

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Poster Presentation : **INOR.P-98**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Cellular Senescence of human Mesenchymal Stem Cells on Silica Nanobeads Surfaces

Yeon-su Yu, Jin Seok Lee*

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All living things experience abnormal phenomena in which the function of the cells that make up the livings decreases and cell division stops permanently, which is called cellular senescence. This phenomenon has been reported to be the biggest cause of genetic damage (DNA damage, telomere dysfunction, tumor gene activation, etc.) caused by various stress-inducing substances (such as active oxygen, radiation, and carcinogens). Human mesenchymal stem cells (hMSC), which can be differentiated into different types of cells (bone cells, fat cells, etc.), age and secrete many chemical factors. This exacerbates the inflammatory response and reduces immune regulatory activity, significantly degrades the differentiation ability and immunity of MSCs, and promotes the growth of cancer cells, thereby promoting tumor production. We want to monitor the functional changes in hMSCs caused by aging, control the cell adhesion and migration through silica nanobeads surfaces, and eventually control cellular senescence. So before we do the study, a system was established to control the senescence of hMSCs through etoposide, an aging-inducing substances. Here, we want to investigate the cellular senescence control of hMSCs through nano-topographic factors of silica nanobeads surfaces.

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Arrangement of electrospun nanofibers according to the length and symmetry of the metal collector

Soo Jin Roh, Jin Seok Lee[*]

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The Electrospinning is a technology that can obtain micro, nano-scale fibers by applying a voltage to a polymer solution. The generated fiber can be used in various fields such as filters and sensors, and in particular, can be used as a biomaterial using a biodegradable material. However, in the case of electrospinning, fiber is formed randomly, so it must be sorted using various methods to effectively use fiber. Therefore, the alignment of fibers is one of the very important factors, and the arrangement of fibers in the gap was confirmed by adjusting the length and symmetry of the collector to find out the mechanism for this alignment. The appearance of the fiber was confirmed using SEM. The orientation of the fiber was confirmed using the Image J program. And to prove the mechanism of deposition tendency, simulation was run using COMSOL program.

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Oxidative Stress mediated cellular senescence in bone marrow mesenchymal stem cells

Nomundelger Gankhuyag, Jin Seok Lee[1,*]

Hanyang University, Korea
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Stem cell senescence is a crucial cause of aging. Time-varying exposure to an oxidative environment mostly impacts cellular senescence along with cellular dysfunction. Mesenchymal stem cells (MSCs) are multipotent cells that can differentiate into a variety of cell types and possess strong capabilities for immunoregulation, and senescent MSCs may lead to inflammation. Their regenerative ability is impaired by cellular senescence. The effects of oxidative stress on MSCs are still unknown. In this study, hMSCs were serially subcultured and cells of two generations (P3 and P8) were observed for reactive oxygen species (ROS) load and senescence parameters including β-galactosidase (β-gal), proliferation potential, and differentiation.Keywords:Cellular senescence, Oxidative stress, DNA damage, Human mesenchymal stem cells

Poster Presentation : **INOR.P-101**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mechanistic Insight on Ir- and Os-Catalyzed Methane Borylation

Yujin Jeon, Bohyun Park, Mu-Hyun Baik*

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The activation and conversion of methane to valuable products has long been a formidable challenge for chemists, given the inherent inertness of its C–H bonds. In 2016, Mindiola and our group reported an Ir-catalyzed methane borylation by utilizing bis(pinacolato)diboron (B_2pin_2) as a boron source.[1] Theoretical studies proposed that the oxidative addition (OA) of methane requires considerable activation energy, stressing the need of catalyst design to achieve catalysis at mild conditions. We successfully improved the catalytic performance by replacing the phenanthroline to the softer bisphosphine ligand, which promotes the rate-determining step. As another strategy, the substitution of the metal center from Ir^{III} to Os^{II} was examined to enhance the catalytic activity of the methane borylation. Delightfully, the Os catalyst showed a promising performance under the room temperature condition. Consistent with our expectations, density functional theory calculations showed a much lower OA barrier for the Os catalyst due to its soft electronics, but it also indicated the presence of a stable intermediate which does not undergo further reaction cycles. The observed yield for Os system was feasible by the kinetic effect of side product HBpin concentration. The shift in reference state made HBpin a key species to determine the rate in Os system, as we can see in the rate equation. Reference[1] Smith, K. T.; Berritt, S.; González-Moreiras, M.; Ahn, S.; Smith III, M. R.; Baik, M.-H.; Mindiola, D. J. Science, 2016, 351, 1424–1427.

Poster Presentation : **INOR.P-102**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Ferroptosis-Apoptosis Hybrid Therapy : A Fenton-Like Reaction Orchestrated Hydroxyl Radical Generation and GSH Depletion in Gastric Cancer

Hyungbin Park, Chaewon Ahn[1], Seungwoo Hong[1,*], Hangil Lee[1,*]

Sookmyung Women's University, Korea

[1]*Department of Chemistry, Sookmyung Women's 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. Apoptosis was also activated by a caspase-dependent pathway in accordance with increasing ROS generation.

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Poster Presentation : **INOR.P-103**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Mixed-valence Bimetallic Metal-organic Framework via Coordinative Reduction

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[1]*Department of Physics & Chemistry, DGIST, Korea*

Bimetallic metal-organic frameworks (MOFs) possess two different metal ions in their framework. Because of the synergistic effects of their two different metal ions, bimetallic MOFs have recently received great interest due to their unique properties and potential applications in catalysis, gas adsorption/desorption, gas separation, and chemical sensing. Meanwhile, controlling the oxidation state of a metal is important because ions have different optic, magnetic, electronic, and catalytic properties depending on their oxidation state. However, the redox activity of metal nodes in MOFs has been rarely examined. Recently, the coordinative reduction method has been investigated as a new method to reduce metal nodes in MOFs. Herein, we reduced the Cu^{2+} metal ion to Cu^{+} in bimetallic paddlewheel MOF containing Cu^{2+} and Ru^{3+} metal nodes using the coordinative reduction method. Only the $Cu^{2+}-Ru^{3+}$ node was reduced to the $Cu^{+}-Ru^{3+}$ node, and the reduction reaction did not proceed further.

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Quantum theoretical study of polyene isomerization by introducing novel derivative of Stone-Wales type transformation especially for buckminsterfullerene C_{60} formation

Hyo Weon Jang

Department of Chemistry, Suncheon National University, Korea

Starting from a particular pure carbon nano cluster like tubelet, ring, or shell, we try to search a plausible reaction pathway to other interesting target cluster. During the investigation, we devise a novel theoretical model isomerization process which is closely related with the well-known Stone-Wales transformation. The present process is characterized by a lower activation energy barrier by almost one-tenth compared to that of the original SW transformation. When the cluster possesses carbene or carbyne moeities, we may deliberately find a suitable intermediate ready for undergoing the present model transformation which is mainly an internal rotation of a rod corresponding to C_2 embedded in the network of hexagons, pentagons, and other polygons composed of sp^2 hybridized C atoms. As an example, we present a quantum calculation of buckminsterfullerene formation reaction pathway starting from a small tubelet derivative of carbon cluster C_{60}.

Poster Presentation : **INOR.P-105**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Binding events of hydroxylase for the C-H activation in soluble methane monooxygenases

Yunha Hwang, Seung Jae Lee*, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

Global warming is a major concern due to climate change from greenhouse gases including carbon dioxide (CO_2) and methane (CH_4). Methane gas is considered the most serious. Although methane gas comprises 8% of greenhouse gas, it has 33 times higher heat capacity than carbon dioxide. Methane monoxide converts methane to methanol and it regulates the level of unavoidable methane gas on the Earth. Soluble methane monooxygenase (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 details of MMOH component interactions with other components including MMOB, MMOR and MMOD, an inhibitory component, will be discussed. The first complex of MMOH-MMOB (PDB: 4GAM) provides crucial information to understand the binding site of MMOH and substrate pathways to diiron active sites. MMOD was considered as a copper binding regulator to control pMMO expression in methanotrophs, but the X-ray structure of MMOH-MMOD demonstrated that MMOD blocked the catalytic cycle through the modification of diiron active sites. This is regulated by the modification of long α-helices of MMOH α-subunit, and structural studies have proved that MMOD 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 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+}.

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Anion Effects on the Construction of Cu(II) Coordination Polymers

Eunbi Jeong, Haeri Lee*

Department of Chemistry, Hannam University, Korea

The reversible oxidation-reduction effect of copper metal ions are fascinating for the field of catalysts and sensors. In order to construct coordination networks including Cu(II), we designed and synthesized a bis(monodentate) N-donor ligand which was fully characterized by 1H, 13C, COSY NMR and mass spectra. Self-assembly of Cu(II) with as-synthesized ligands gives rise to six different type of Cu(II) complexes depending on anions and reaction conditions. Their crystal structures were fully characterized by single crystal X-ray diffractometer. Mainly, the coordination environment for Cu(II) plays a key role in its skeletal structure. The further research on the structural effects of Cu(II) networks are undergoing.

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Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

4-Nitrophenol Sensing using Zn(II) Coordination Polymers

HyunSeo Kim, Hyemin Lee, Haeri Lee[*]

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-108**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

RuxCr1-x nanoparticles encapsuled Carbon nanofibers for bifunctional electrocatalytic Overall water splitting

Myung Hwa Kim*, Chongmok Lee[1,*], Dasol Jin[1], Ji Won Kim[2]

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

Electrocatalytic water splitting into hydrogen and oxygen is a promising way to solve the energy crisis and achieve sustainable energy conversion and storage. Generally, the water splitting is divided into two half reactions, the oxygen evolution reaction (OER) at the anode and the hydrogen evolution reaction (HER) at the cathode. These reactions require high overpotential and has low stability. Therefore, it is necessary to develop a high performance electrocatalyst, which has lower kinetic barrier of OER, increase activity of HER and greatly improve the energy efficiency. The state-of-the-art electrocatalysts for both OER and HER mostly depend on noble metals such as iridium (Ir) and ruthenium (Ru). However, due to the high price and scarcity of noble metal-based catalysts, developing bifunctional electrocatalysts for overall water splitting is limited.In this study, thus, we incorporated Chromium (Cr) into Ruthenium (Ru) to form the high-crystalline single phases of RuxCr1-x Nanoparticles on Electrospun Carbon Nanofibers via one-step electrospinning process followed by the thermal annealing. We carefully examined the formation of bimetallic phases on Carbon nanofibers in terms of various compositions and annealing temperature in order to optimize the electrochemical performances in both OER and HER. Furthermore, we explore pH-universal electrocatalytic performances of both OER and HER in the broad range of pH.

Poster Presentation : **INOR.P-109**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Oxidation of Aniline Derivatives by Coordinatve Reactions in HKUST-1 with Hydrolytic Stability Enhancement

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. Aniline, containing amine groups which strongly bind at open metal sites, can give metal nodes an electron in MOF by ligand to metal charge transfer (LMCT), then forms bond to be an azobenzene. 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. In addition, different functional groups in aniline derivatives are treated for investigating the effect of electron donating/withdrawing groups to LMCT reaction in HKUST-1.

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

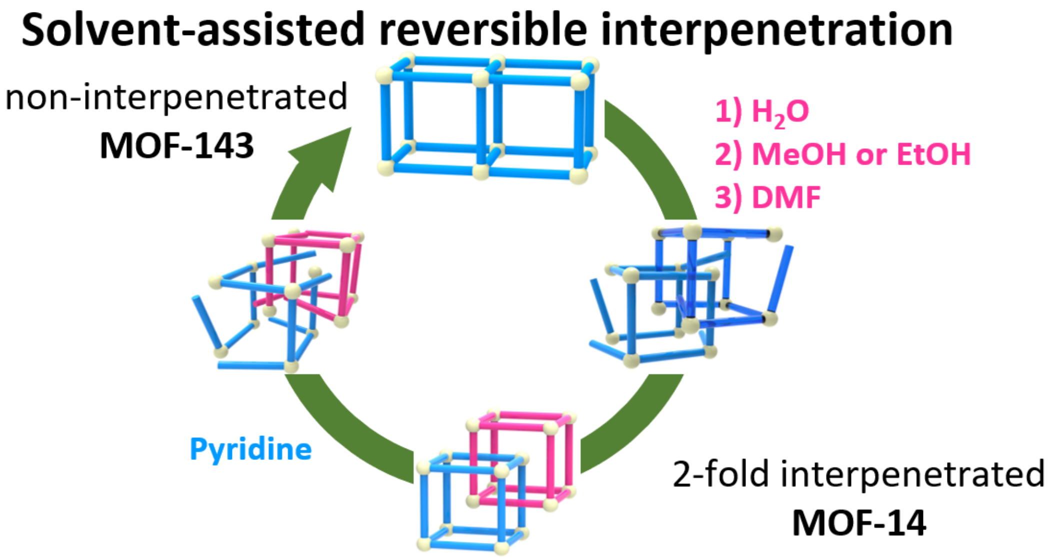
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Solvent-assisted Reversible Interpenetration and De-interpenetration of a Cu-Paddlewheel-Based Metal-organic Framework and Its Ethane Uptake

Cheol Yeong Heo, Nak Cheon Jeong*

Department of Physics & Chemistry, DGIST, Korea

We report 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. Adsorption isotherms of ethane and ethylene were measured at 298 K and up to 1 bar to find that pristine MOF-14 exhibited remarkable ethane uptake (71 cm^3 g^{-1}) and a modest selectivity of ethane over ethylene.



Poster Presentation : **INOR.P-111**

Inorganic Chemistry

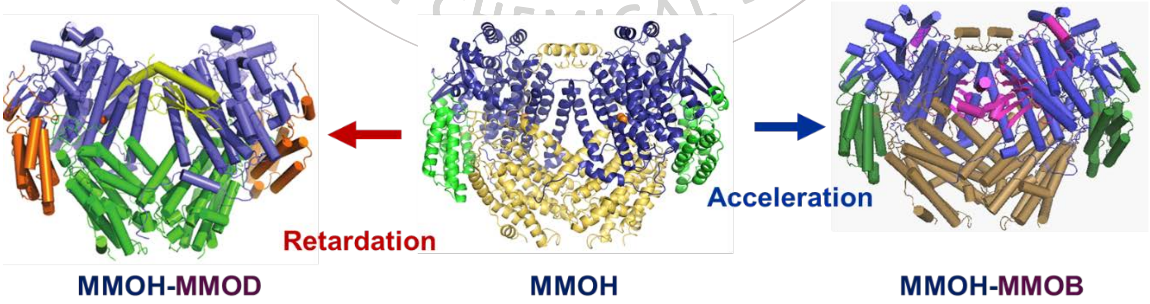
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Complex generation of MMOH with other components

Yunha Hwang, Seung Jae Lee*, Dong-Heon 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.



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Poster Presentation : **INOR.P-112**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Carboxylate Metal-Organic Framework Glass

Minhyuk Kim, Hoi Ri Moon[1,*]

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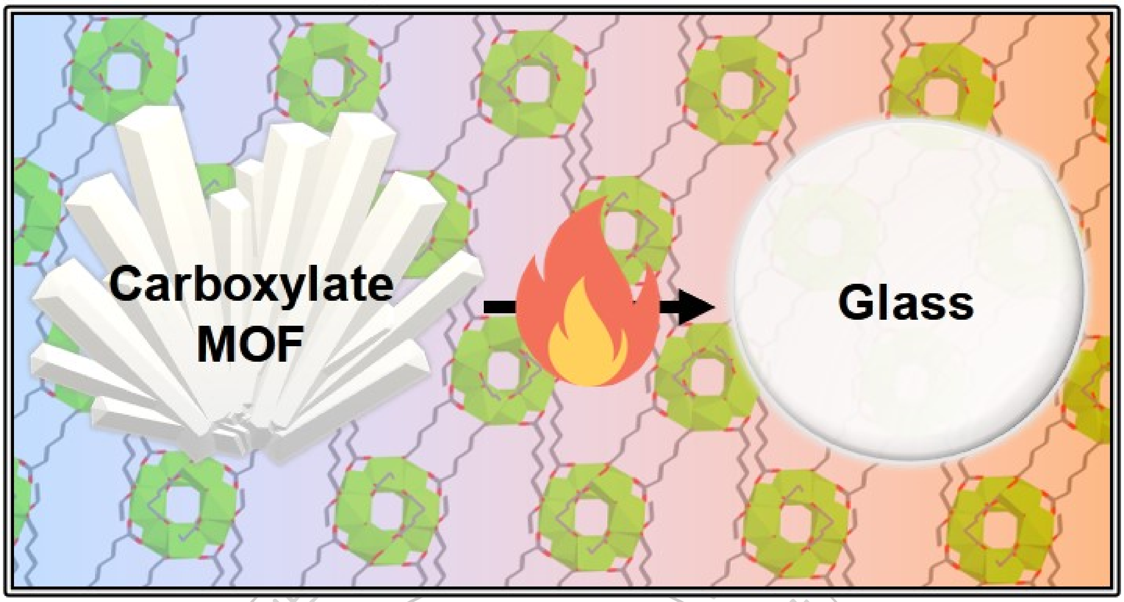
[1]*Department of Chemistry and Nanosciecne, Ewha Womans University, Korea*

Despite the fact that carboxylate-based frameworks are commonly used architectures in metal-organic frameworks (MOFs), reported liquid/glass MOFs have been obtained from azole- or weak coordinating ligand-based frameworks. Hitherto, the strong coordination bonds of carboxylate ligands to metals were known to block the thermal vitrification pathway of MOFs. Here, we report the first example of carboxylate-based melt-quenched MOF glass, which is composed of magnesium and an aliphatic carboxylate ligand, adipate (adp). This MOF has a low melting temperature (Tm) of 284 °C, compared to 3D azole-based MOFs, and a high glass-forming ability of 0.92. The flexibility and low symmetry of the aliphatic carboxylate ligand and a lack of ligand field stabilization energy on Mg2+ can contribute to a decreased Tm, resulting in the melting of carboxylate-based MOFs. Nanoindentation test reveals that this glass MOF has superior mechanical properties in hardness (H) and elastic modulus (E). Our research is the first step of carboxylate-based MOFs sheds light on the viability of various meltable carboxylate-based MOFs.

Melt-Quenching



Poster Presentation : **INOR.P-113**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation of Zn-MOFs with bpe & AZPY and their antifungal application.

Seo yeon Heo, **Suk Joong Lee**[1,*]

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

As concerns related to human inflammation deepen, research on the application of MOF is continuously being conducted. Herein, two 3D Zn-MOFs containing glutarates and 1,2-bis(4- pyridyl)ethylene (bpe) or 4,4'-azopyridine (AZPY) were synthesized and their structures were analyzed by using X-ray crystallography. As a result, the solvothermal reaction provides the similar structure for both Zn-MOFs containing bpe (1-bpe) or AZPY (2-AZPY). The coordination environment of a Zn(II) ion is distorted tetrahedral constructed by three carboxylate oxygen atoms from three different carboxylates and one nitrogen atom from bpe or AZPY. In addition, we analyzed the antifungal activities of Zn-MOFs against filamentous fungi, *Cladosporium cladosporioides (C. cladosporioides)* and *Aspergillus niger (A. niger)* and a yeast, *Candida albicans (C. Albicans)*. 2-AZPY shows better antifungal activity by released AZPY from 2-AZPY than 1-bpe. The released AZPY ligands can deactivate fungal cells by interacting with thiol groups of proteins to produce S-S coupling. Due to its great antifungal activity, Zn-MOF containing AZPY may have an outstanding sanitary applications.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication of Porphyrin embedded nanofibers and their antibacterial Activities

Daeyong Kim, Suk Joong Lee[1,*]

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

As COVID-19 has shown a great danger of infection and secondary contamination, the antibacterial and antiviral studies have become one of the most important research areas. Bacteria and virus in natural surroundings must be eliminated before their penetration into human bodies as they proliferate and propagate in cells, causing serious damages. Therefore the study is mainly focused on eliminating residual bacteria and viruses on surroundings and developing suitable antibacterial systems. In this research, the proactive bacterial elimination is materialized by fiber based photosensitizer. A well-known photosensitizer, porphyrin which absorbs visible light and produce reactive oxygen species is crosslinked in PVA nanofiber. The photocatalytic ability was tested and actual antibacterial activity was assessed with in vitro anti-bacterial experiments. Bacteria-containing solution is treated with porphyrin embedded nanofiber and exposed to UV light to incur antibacterial reaction.*E. Coli* and *L. Innocua* were chosen to compare antibacterial ability of synthesized fibers against gram negative and positive bacteria.

Poster Presentation : **INOR.P-115**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

SOD mimicking Copper Complex for Triple Negative Breast Cancer Therapy

Chaewon Ahn, Hyungbin Park, Seungwoo Hong*, Hangil Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Having a significant impact on current cancer chemotherapy is the development of metal complexes with platinum central atoms such as cisplatin or carboplatin. 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. Promising as anticancer agents are copper complexes among non-Pt compounds. For many years, research has actively investigated copper compounds based on the proposal that endogenous metals may be less toxic. Copper is found in all living organisms and is a crucial trace element in redox chemistry, growth, and development. The major functions of copper biological molecules involve oxidation–reduction reactions in which they react directly with molecular oxygen to produce free radicals.When MDA-MB-468, triple-negative breast cancer cell, was treated with [M(bsc-Bn)]$^{2+}$ (M=Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}), the most effective and toxic complex with a low concentration among [M(bsc-Bn)]$^{2+}$ complexes is [Cu(bsc-Bn)]$^{2+}$. It was found that [Cu(bsc-Bn)]$^{2+}$ complex could effectively function as the role of disproportionation of superoxide in cancer cells. Also, the formation of ATP is suppressed, and cell cycle arrest occured to induce apoptosis of MDA-MB-468.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile Fabrication of Defect-Free Metal-Organic-Frameworks(MOFs) Membranes via Interfacial Synthesis

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Membrane-based separations are considered energy-efficient alternatives to replace the existing energy-intensive distillation by eliminating the thermally driven phase change step. As membrane materials, polymers have been used primarily because of their cost-effectiveness and mechanical adaptability, but their poor permeability and selectivity have been a major challenge. To overcome these problems, researchers have shifted their attention to crystalline nanoporous membranes as promising candidates, especially metal-organic frameworks (MOFs)- based membranes which exhibit both high selectivity and permeability. For decades, many interesting results of MOF-based high-performance membranes have been published, proving their potential as high performance membrane. However, there are still many challenges, such as the formation of nonselective defects, weak substrate binding affinity, and time-consuming multistep procedures. In this study, we present a simple one-step method for fabricating defect-free MOFs (HKUST-1, ZIF-8, and MIL-88A) membranes via interfacial synthesis utilizing porous anodic aluminum oxide (AAO) substrate. Using this simple strategy, defect-free MOF membranes can be easily prepared in a short time under mild conditions, even at room temperature. The prepared membrane was characterized by infrared spectroscopy(IR), powder x-ray diffraction (PXRD), and scanning electron microscopy(SEM), and we confirmed its performance through a dye separation test that demonstrated the absence of any defects in the membrane assembly.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis Approaches of New Heteroleptic Zr- and Hf-Aminoalkoxide Precursors for Atomic Layer Deposition

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

Zr- and Hf-oxide thin films are of utmost interest for future generation high-tech applications, for instance, regarding Metal-Insulator-Metal (MIM) structures in memory applications. Many techniques have been evolved for the synthesis of respective precursors, however, the most challenging task is still to design a precursor with the well-known desired features, such as sufficient volatility, thermal stability, and reactivity. Introduced herein are synthesis approaches for the design of new heteroleptic Zr- and Hf-precursors by the inclusion of aminoalkoxide ligands based on our previous studies. Reactions conducted were monitored by ^{1}H- and ^{13}C-Nuclear Magnetic Resonance (NMR) and Fourier-Transform Infrared Spectroscopy (FT-IR).

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Multi-metal Adjustment Capability of Fe-scorpionate Systems

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chemistry, Chonnam National University, Korea
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The term "scorpionate" was introduced in the 1960s after Tropimenko reported tris (pyrazolid) borate.[ref1] In modern times, Scorpio is one of the most widely studied coordination compounds in coordination chemistry. Scorpionate have characteristics such as metal ion control, metal exchange, etc., and are used in supramolecular, polymer chemistry, homogeneous catalysts, etc.Our lab uses Fe(III) as the central metal and reports scorpionate compounds of [O,N] chelate ligand, 5-(2-hydroxyphenyl)-1H-tetrazole.[ref2] In our system, three nitrogen from tetrazole and three oxygen from phenol form a triangular shape facing one side at different angles. The parts of this triangle bind to metal ions.In order to test the capability of the metal control system, scorpionate ligands were synthesized using alkali metals (Li, Na, K, Cs, Rb) alkaline earth metal salts (Mg, Ca, Sr, Ba), and the combination of scorpionate ligands and metals was different depending on the type of metal used. In the case of K, it was confirmed that only a scorpionate ligand exists without the combination of the scorpionate ligand and Mg, whereas in the case of Mg, only a scorpionate ligand exists. In the case of Ca, it was confirmed that two types were selectively synthesized according to the equivalent ratio. We identified a complex that binds O- and N-sites of two Scorpio ligands in κ2 coordination mode. Ba was stabilized by a solvent by taking the κ3 coordination mode up to the O site of the Scorpio ligand. The binding method was investigated through X-ray crystallography, and the compounds obtained by various analysis methods were identified.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mechanical Properties Analysis of Metal–Organic Frameworks (MOFs) Using Atomic Force Microscopy

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Metal–organic frameworks (MOFs) consist of metal ions or clusters coordinated by organic linkers designing unique structures and properties. These are in the spotlight for various uses, such as gas storage and separation, sensing, and catalysis [1]. The functionality of MOFs is engineered by incorporating specific ligands with desired functional groups and interpenetrating two or more frameworks towards the attained framework dynamics and well-defined pores [2]. X-ray diffraction and electron microscopy techniques have characterized MOF structures [3]. However, specific measurement environments are required, limiting the observation of native functions of MOF structures. Here, we utilize atomic force microscopy (AFM) as a high-resolution characterization tool in liquid phases, retaining MOF functions and structures. We observe nanomechanical interactions between the AFM probe and Zr-based UiO-type MOF surfaces with different degrees of interpenetration (DOI). These measurements allow more accurate investigations into elastic modulus and framework deformations of MOF compounds in the stable interfaces to understand their original functionality.Reference[1] Kreno, L. E. et al. Chem. Rev. 2012, 112, 1105-1125.[2] Zhang, Y. et al. Angew. Chem. Int. Ed. 2019, 131, 8229-8234.[3] Robison, L. et al. J. Am. Chem. Soc. 2021, 143, 1503-1512.

Poster Presentation : **INOR.P-120**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ligand Control to Modified Various Structures of Strontium Complexes

Chanwoo Park, Taek-Mo Chung[1,*]

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Group 2 metals such as calcium, barium, and strontium, especially the latter on, are attractive elements because of their variety of applications like e.g. in optical waveguides, electrically tuneable microwave devices, colossal magnetoresistive thin films, or metal-insulator-metal (MIM) capacitors. In these fields, fabrication of thin film containing strontium oxides is required which can be deposited by various ways such as metal-organic chemical vapour deposition (MOCVD), or atomic layer deposition (ALD). To apply these deposition techniques, strontium precursors exhibiting volatility and thermal stability are essential. However, the synthesis of suitable compounds for the deposition of strontium oxides is limited due to their tendency to form oligomeric complexes which can be attributed to their large radius, small charge, and high coordination number. To prevent oligomerization, we introduced bulky and multidentate ligands. In this study, we produced heteroleptic complexes using pentadentate aminoalkoxide ligands and β diketonate ligands to prevent the formation of oligomeric complexes. New strontium β-diketonate complexes were synthesized by the substitution reaction of the bis(trimethylsilyl)amide of Sr(btsa)2·2DME with an ethereal group and β-diketonate ligands. The compounds [Sr(tmge)(btsa)]2 (1), [Sr(tod)(btsa)]2 (2), Sr(tmgeH)(tfac)2 (3), Sr(tmgeH)(acac)2 (4), Sr(tmgeH)(tmhd)2 (5), Sr(todH)(tfac)2 (6), Sr(todH)(acac)2 (7), Sr(todH)(tmhd)2 (8), Sr(todH)(hfac)2 (9), Sr(dmts)(hfac)2 (10), [Sr(mee)(tmhd)2]2 (11), and Sr(dts)(hfac)2 (12) were obtained and analyzed by various techniques, including FT-IR, NMR, TGA (Thermogravimetric analyses), and elemental analysis.

Poster Presentation : **INOR.P-121**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Novel Tin(II) sulfide Complexes for 2D Semiconductor Materials

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Tin monosulfide (SnS) is potential material for next-generation photovoltaic cells and has good properties for solar cells such as an ideal mid-range direct band gap (ca. 1.3 eV), high optical absorption coefficient (>10^4 cm-1), p-type conductivity, low cost, non-toxic, and earth-abundant elements. However, the power conversion efficiency of SnS-based photovoltaics is still low, less than 5%. In order to promote the process for the tin(II) sulfide, suitable precursors are necessary. So, we successfully synthesized a series of novel tin compounds with the aim of enhancing the interaction ability between the Sn metal center and the S derivative to increase the thin film deposition efficiency.All synthesized complexes were fully characterized by NMR, FT-IR spectroscopy, elemental analysis and thermogravimetric (TG) analysis. In particular, the thermal plot of the complexes showed that the residual mass was consistent with the ideal SnS mass value at 600 °C. These results suggest that the complexes are stabilized by *S,O*-chelate binding effect with the N-alkoxy thioamide derivative ligand.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Controlled assembly of gold nanocubes

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Self-assembly of nanoparticles can be a facile, controllable, and scalable bottom-up strategy for fabricating desired nanostructures. While many previous methods have largely controlled forces between particles through ligands and physical and chemical stimuli, these studies have limitations, such as limited material selection or the use of a fluidic template. Thus, advanced methods in nanoparticle assembly are required for future applications. In this study, we discuss synthesis and assembly of gold nanocubes, especially in controlled morphology and crystalline structure. Prepared well-ordered lattice structures that are scalable and widely applicable could be presented with the representative case of gold nanocubes structure. Highly ordered, crystalline plasmonic assemblies formed could open new ways for further applications, including optics, sensing, imaging, and catalysis.

Poster Presentation : **INOR.P-123**
Inorganic Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Novel Ru Precursors for Atomic Layer Deposition

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Ruthenium (Ru) is a popular metal for various applications in the state of-art semiconductor device technologies, due to their properties such as chemical stability, thermal stability, low resistivity(~7 μΩ cm), and a large work function(～4.7 eV). It is mainly used as a material for seed layer of copper electroplating, capacitor electrode in dynamic random access memory (DRAM) devices and a metal gate of metal-oxide semiconductor field effect transistor (MOSFET). Therefore, research on Ru thin films, that can be deposited by methods such as MOCVD (Metal-Organic Chemical Vapor Deposition) and ALD (Atomic Layer Deposition), is attracting many researchers. To apply these deposition techniques, Ru precursors with volatility and thermal stability are required. In this study, for the synthesis of Ru precursors that can satisfy all conditions, new Ru precursors were designed and prepared by using Ru(η5-Tropone)(η5-CHT) (CHT = Cycloheptatriene) as a starting material, to yield five new ruthenium precursors: Ru(II)(C7H9)(C8H11O) (1), Ru(II)(C7H9)(C9H14O) (2), Ru(II)(C7H9)(C13H14O)(3), Ru(II)(C7H9)(C8H9O) (4), and Ru(II)(C7H9)(C9H11O) (5). These compounds were characterized by 1H-Nuclear Magnetic Resonance (NMR), Mass Spectrometry (MS), Fourier-transform Infrared Spectroscopy (FT-IR), Elemental Analysis (EA), Thermal Gravimetric Analysis (TGA), and single crystal X-ray diffraction.

Poster Presentation : **PHYS.P-124**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Isotherm models for VOCs adsorption released from the fiber-reinforced plastic production

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Materials and Energy Centre, Agency for Defense Development, Korea

The utilization of isotherm techniques in the examination of volatile organic compounds (VOCs) in fiber-reinforced plastic production has gained widespread recognition as they furnish valuable insights into the nature of the adsorption process and the interactions between the VOCs and the adsorbent material. Through the utilization of isotherm techniques, various crucial parameters can be determined, including the maximum adsorption capacity, the energetics of the adsorption mechanism, and the type of isotherm. Additionally, isotherm techniques offer a quantifiable method for evaluating the efficacy of various adsorbent materials in terms of their ability to adsorb VOCs, which is imperative in selecting the most suitable adsorbent material for practical applications, such as air purification or remediation of contaminated sites.

Poster Presentation : **PHYS.P-125**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory for Accurate X-ray Absorption Spectroscopy

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It is demonstrated that the challenging core-hole particle (CHP) orbital relaxation for core electron spectra can be readily achieved by the mixed-reference spin-flip (MRSF)−time-dependent density functional theory (TDDFT). With the additional scalar relativistic effects on K-edge excitation energies of 24 second- and 17 third-row molecules, the particular ΔCHP−MRSF(R) exhibited near perfect predictions with RMSE ～0.5 eV, featuring a median value of 0.3 and an interquartile range of 0.4. Overall, the CHP effect is 2−4 times stronger than relativistic ones, contributing more than 20 eV in the cases of sulfur and chlorine third-row atoms. Such high precision allows to explain the splitting and spectral shapes of O, N, and C atom K-edges in the ground state of thymine with atom as well as orbital specific accuracy. The same protocol with a double hole particle relaxation also produced remarkably accurate K-edge spectra of core to valence hole excitation energies from the first (nO8π*) and second (ππ*) excited states of thymine, confirming the assignment of 1s → n excitation for the experimentally observed 526.4 eV peak. Regarding both accuracy and practicality, therefore, MRSF−TDDFT provides a promising protocol for core electron spectra of both ground and excited electronic states alike.

Poster Presentation : **PHYS.P-126**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combi-ned with Mixed-Reference Spin-Flip TDDFT

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[1]*Aix-Marseille Univ, France*
[2]*Department of Chemistry, Kyungpook National University, Korea*

The photochemistry of nucleobases, important for their role as building blocks of DNA, is largely affected by the electrostatic environment in which they are soaked. For example, despite the numerous stud-ies 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 embeddingQM/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. For the thymine dimer in B-DNA, we found new photochemical pathways through conical intersections that could explain the formation of cyclobutadiene dimers and 6−4 photoproducts.


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Poster Presentation : **PHYS.P-127**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Prototropically Controlled Dynamics of Cytosine Photodecay

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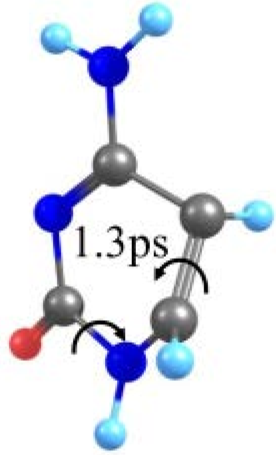
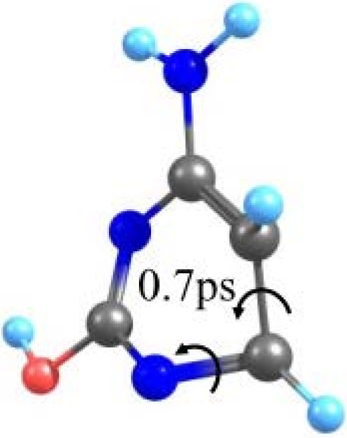
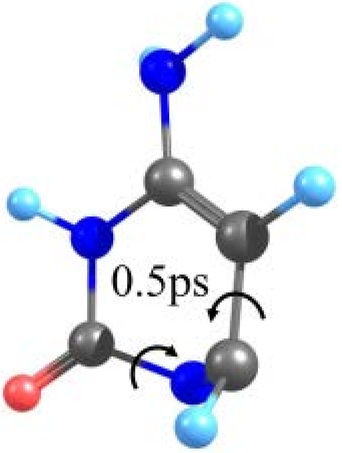
The effect of the existence of several prototropic tautomers of cytosine on its UV/vis spectra and the excited state decay dynamics is studied by spectral and nonadiabatic molecular dynamics (NAMD) simulations in connection with the mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) method. Simulated UV/vis spectra provide a strong indication that the H3N keto–amino cytosine tautomer (the least anticipated species) may be present under experimental conditions. The NAMD simulations yield a wide range of excited state decay constants for various tautomers of cytosine, ranging from ～1.3 ps for the biologically relevant H1N keto–amino tautomer to ～0.1 ps for the keto–imino tautomer. The slowness of the H1N decay dynamics follows from the presence of a barrier on the excited state energy surface separating the Franck–Condon structure from the major decay funnel, the conical intersection seam. It is suggested that the experimentally observed photodecay dynamics may result from a combination of the decay processes of various tautomers (H3N in particular) present simultaneously under the experimental conditions.



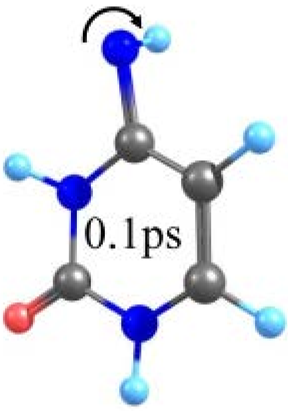
keto-amino (H1N)



enol-amino



keto-amino (H3N)



keto-imino

Poster Presentation : **PHYS.P-128**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Excited States Dynamics Studies of Thiouracil including Intersystem Crossing via Time-resolved X-ray Absorption Spectroscopy

Seong Hyeon Jeong, Tae Kyu Kim[1,*]

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

Uracil is the one of nucleobases in the RNA, which has inherent photo-protective mechanism to prevent from harmful UV radiation. In specifically, when UV light is radiated to uracil, the excited state relaxation occurs very fast along the singlet pathways. However, thionation of exocyclic oxygen to sulfur can change this inherent biochemical feature to a new one. 2-thiouracil has large spin-orbit coupling between the excited singlet and triplet states, so intersystem crossing happens more dominantly in thiouracil than uracil. The excited triplet states decay to ground state slowly and have high reactivity so that it could be used to biotherapeutic ways. In this regard, we report time-resolved x-ray absorption spectroscopy results to study excited state dynamics of 2-thiouracil and 2,4-dithiouracil and plan to analyze UV excitation decay dynamics. S1(nπ*) state is optically blind dark state so that transient absorption spectroscopy can not see the forbidden S1 state. But the x-ray probes, especially S K-edge can directly probe elemental specific electronic structure near S atom environment. So, we expect to trace the non-adiabatic internal conversion from S2(ππ*) to S1 at the conical intersection of two potential energy surface, or intersystem crossing to triplet ππ* or nπ* states.

Poster Presentation : **PHYS.P-129**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

In-situ XPS study for Photocatalytic Performance Variations of ZnxCd1-xS Nanoparticles Depending on Irradiated Wavelength

Vy Pham, Hyun Sung Kim[1,*], Hangil Lee[2,*]

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[1]*Department of Chemistry, Pukyong National University, Korea*
[2]*Department of Chemistry, Sookmyung Women's University, Korea*

Photocatalysts are useful for various applications, including the conservation and storage of energy, wastewater treatment, air purification, semiconductors, and to produce high-value-added products. Herein, ZnxCd1-xS nanoparticles (NPs) with different concentrations of Zn2+ ions were successfully fabricated. In-situ X-ray photoelectron spectroscopy (XPS) was performed to investigate the effect of the Zn vacancies on the irradiation wavelength for photocatalytic activity. Furthermore, wavelength-dependent photocatalytic degradation (PCD) activity of the ZnxCd1-xS NPs was investigated using 2,5-hydroxymethylfurfural (HMF). We observed that the selective oxidation of HMF resulted in the formation of 2,5-furandicarboxylic acid (FDCA) depending on the irradiation wavelength for PCD.

Poster Presentation : **PHYS.P-130**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tracking Charge-Carrier Dynamics of Solid-State Photocatalysts with Femtosecond Time-resolved X-ray Absorption Spectroscopy using XFEL.

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Transition metal oxide is one of the promising candidates for solar energy conversion and photocatalysts. However, dynamic changes by the surface structures have not been elucidated well. Here, we used a femtosecond X-ray absorption spectroscopy to investigate the electron dynamics between TiO_2 and surface engineered blue TiO_2. We observed the changes of electronic and structural change of Ti 3d orbitals and charge transfer dynamics. In the static analysis, we observed difference at pre-edge region which means structural and electronic change. We confirmed that the distorted structure by oxygen vacancies in blue TiO_2 increase A2 peak at the pre-edge region. With the time-resolved experiment, we identified one positive feature at the pre-edge region and two positive peaks at edge region. At the pre-edge region, the rising and decay components were similar in both TiO_2 and blue TiO_2. At the edge region, we observed the 2 components for TiO_2 and 1 component for blue TiO_2. The oxygen vacancies in the surface showed little effect to electrical and structural change rate but they induced difference in charge transfer mechanism between two samples. Using the time-resolved X-ray absorption spectroscopy (TRXAS), we directly investigated electron dynamics of TiO_2 and blue TiO_2. We expect that the dynamic information can suggest a direction for designing catalyst system.

Poster Presentation : **PHYS.P-131**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

High-reliable and Large-scale simulations of Promising Argyrodite Solid-State Electrolytes using Machine Learned Moment Tensor Potential

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Nowadays, solid-state electrolyte (SSE) is being immensely researched as one of the solutions to significantly solve safety issues and increase energy density for next-generation batteries. Then, we focused on a sulfide-based argyrodite (Li_6PS_5X (X=Cl, Br, I)) as a promising SSE material due to its comparable Li-ion conductivities to liquid electrolytes. In general, most computational SSE studies are conducted by the ab initio molecular dynamics (AIMD), which features higher accuracy. However, when we compared the experimental result, there are problems such as the difference in ionic conductivities (σ_{RT}), relatively small cell size and time cost. Herein, to overcome the above drawback, we calculated that the moment tensor potential (MTP) which is one of the machine-learning potentials can be significantly applied for SSE research due to its time efficiency and expectation accuracy by the training sets of AIMD results. Then, we systematically designed a 3x3x3 Li_6PS_5X cell structure, which has randomly dispersed 4a, and 4c sites to represent like experiment structures and obtain similar results (eq. σ_{RT}) as contrasted experimental results. σ_{RT} of the structure is 2.15 mS cm^{-1} at 80% crystallinity, which is a highly accurate result compared to the experiment result (1-3mS cm^{-1}).). Additionally, we unveil that the higher σ_{RT} of argyrodite is related to the vibrational motion of the PS_4 polyhedron rather than its rotational motion. Based on these theoretical investigations, we believe that our results not only give insight into the various argyrodite composition studies but also incredibly improve time cost-efficiency.

Poster Presentation : **PHYS.P-132**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Spatiotemporal carrier dynamics of pyrene incorporated multi-cation halide perovskites with high stability

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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.

We observed further device stabilization of $Cs_x(FAPbI_3)_{0.95}(MAPbBr_3)_{0.05}$ perovskites by incorporating pyrene molecules in the precursor 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. Pyrene molecules were found to increase the diffusivity rate by a fold of 2 and therefore greatly enhancing the diffusion length. This proves 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 of perovskite films when exposed to moisture. Perovskite with pyrene addition showed no degradation in grain morphology and slower formation of nonradiative recombination sites near the grain boundaries.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **PHYS.P-133**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ultrafast Intersystem Crossing of Ru Complexes for Photosensitizer

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

Dye-sensitized solar cells (DSSCs) have emerged for their ease of fabrication and stability. However, despite these advantages, DSSCs are still under research due to their low photovoltaic conversion efficiency. This efficiency can be increased in several ways, notably by using different sensitizers that are more inclined to donate electrons to the semiconductor. Because the charge transfer effectively occurs at the sensitizer's triplet excited states, its intersystem crossing (ISC) rate competing with internal conversion (IC) will be an important factor for the efficiency. In this study, we illustrate the photochemical relaxation dynamics of four different archetypical molecules, homoleptic complexes $[Ru(bpy)_3]^{2+}$, $[Ru(bpz)_3]^{2+}$ and heteroleptic complexes $[Ru(bpy)_2(bpz)]^{2+}$, $[Ru(bpy)(bpz)_2]^{2+}$ by using the surface hopping method which is a mixed quantum-classical simulation technique. We found slower ISC from singlet to triplet in heteroleptic complexes (provide time scale) compared to the homoleptic complexes (provide time scale). Following normal mode analysis and charge density analysis suggests that the relaxation pathway of the heteroleptic complex involves stepwise relaxation of bipyrazine and bipyridine ligands. In addition, transient absorption spectra are simulated to provide experimentally observable quantity.

Poster Presentation : **PHYS.P-134**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mechanisms of Carbonic Anhydrase and its Metal Variants through DFT Calculations

Rajeev Kumar, Jeong-Mo Choi*

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, 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 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 depend on the identity of the metal.

Poster Presentation : **PHYS.P-135**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Role of electrostatic interactions in phase separation of gephyrin

Da-Eun Hwang

Department of Chemistry, Pusan National University, Korea

Liquid-liquid phase separation (LLPS) of biomolecules has recently attracted broad interest due to its role in the spatiotemporal compartmentalization of eukaryotic cells. Postsynaptic density (PSD) is a protein complex composed of hundreds of proteins located on the surface and inside of the postsynaptic membrane of excitatory synapses. It was shown that various scaffolding proteins in excitatory synapses form PSD through LLPS. Among them, gephyrin is the core scaffolding protein in inhibitory PSDs, and it consists of two folded domains and a large unstructured linker that connects the two. Recently, the mechanism of gephyrin clustering in PSDs through liquid-liquid phase separation was experimentally elucidated. However, the molecular mechanism behind this collective behavior is yet unclear. We used atomistic Monte Carlo simulations on the wild-type and mutant gephyrin systems to obtain molecular insights and found that the electrostatic interactions between the basic residues on the disordered linker and the acidic residues on the folded domains are critical for determining the structural ensemble. We hypothesize that the same electrostatic interactions are the driving force of gephyrin LLPS, which leads to the prediction that perturbation of the key residues will decrease the LLPS propensity.

Poster Presentation : **PHYS.P-136**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Understanding the effects of polarizability of Li cations and PEO chains on the diffusion and structure in PEO electrolyte systems by using molecular dynamics simulations

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

The polarizability of the molecules may affect the physical properties of Li-polymer electrolyte systems and is caused by the induced dipole moment of Li^+ ions and polymer chains. However, most molecular dynamics simulations ignored the polarizability of molecules because of expensive computational costs. We perform all-atom molecular dynamics simulations with APPLE&P force field, which allows us to turn on and off the polarizability systematically. We employ PEO polymer electrolytes composed of 10 chains of PEO with 54 EO monomers and 54 LiTFSI salts. We find that the coordination between Li^+ ions and PEO chains and the aggregation of PEO chains are affected by the polarizability, with the polarizability of PEO chains having the most significant impact on the structure. If polarizability is considered properly, the coordination number ranges from 5 to 6. With polarization ignored, the coordination number decreases significantly. In addition to these structure differences, the diffusion of Li^+ ions is much faster with polarizability. This result indicates that the polarizability of molecules affects the correlated motion of Li^+ ions and PEO chains, with the aggregation of PEO chains and the coordination numbers playing a role in determining the diffusion.

Poster Presentation : **PHYS.P-137**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Reaction mechanism study of Aza-Brook rearrangement using Computational Chemistry

Ka young Cho, Won-SuK Kim[1], Jiyong Park[2], Jaehong Park*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Chemistry Department of Nano-Science, Ewha Womans University, Korea*
[2]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

The Brook rearrangement is one of the most important reactions in synthetic chemistry. Here's a Brook rearrangement (or aza-Brook rearrangement) with two possibilities: [1,3] shift and [1,5] shift. However, as is well known, it is difficult to experimentally determine the mechanism of these organic reactions. Therefore, we tried to reveal the mechanism through computational chemistry. Density Functional Theory was used, and geometry optimization and single-point energy calculation were conducted. We hope that this research will lead to further applications.

Poster Presentation : **PHYS.P-138**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Percolation-Based Unifying Description of Liquid-Liquid Phase Separation and Gelation of Associative Polymers

Da-Hyun Koo

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 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 liquid-liquid phase separation and gelation in the language of graph theory; liquid-liquid phase separation can be depicted by emergence of a giant component, whereas gelation is defined by the diffusion behavior. We introduced *dwell time* to quantify the diffusion behavior of the system, and it could be demonstrated that the dwell time correlates well with the size of the giant component. We also found that there are two relaxation processes, fast and slow; the former can be thought of as initial formation of small clusters (protocondensates or seeds), while the latter displays phase separation. Our study demonstrates that such a simple model can provide qualitative understanding of an apparently complex biological phenomenon.

Poster Presentation : **PHYS.P-139**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Cooperative Effect of Nickel ferrite (NiFe2O4) Underlayer and Amorphous Nickel Iron Oxide (NiFeOx) Overlayer on the Cathodic Shift of the Onset Potential for Water Oxidation on Hematite (α-Fe2O3) Photoanode

Nakyung Lee, Woon Yong Sohn[1,*]

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We fabricated a Hematite-based photoanode, treated by both a Nickel ferrite (NiFe2O4) underlayer and an amorphous Nickel iron oxide (NiFeOx) overlayer, and investigated the effect of the treatments on the photo-electrochemical (PEC) water oxidation. In this study, we found that introducing the underlayer had a negative effect on the PEC performance, particularly, in terms of onset potential. On the other hand, a cathodic shift could be achieved when the overlayer and underlayer were introduced at the same time, which was larger than that of the single treatment of the overlayer. We will discuss the origin of cooperative effect of the underlayer and the overlayer on the cathodic shift of the onset potential for water oxidation on hematite photoanode, based on the results obtained by various electrochemical and spectroscopic techniques.

Poster Presentation : **PHYS.P-140**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A New Strategy for Monitoring the Charge Transfers from Perovskite Thin Films to Electron Transport Layers using Heterodyne Transient Grating Technique

Young Hyun Kim, **Woon Yong Sohn**[*]

Department of Chemistry, Chungbuk National University, Korea

We fabricated CH3NH3PbI3 (MAPbI3) thin films with and without a ZnO layer and measured heterodyne transient grating (HD-TG) responses of each film to investigate the charge injection dynamics from MAPbI3 to ZnO, based on the component arising from the recombination of the surface trapped electrons in the ZnO layer with the remaining holes in MAPbI3. In addition, we observed the HD-TG response of the MAPbI3 thin film coated with the ZnO layer in which Phenethyl ammonium iodide (PEAI) was inserted between two layers as a passivation layer and confirmed that the charge transfer was enhanced when PEAI existed, based on the increase in the amplitude of the component arising from the recombination and its acceleration.

Poster Presentation : **PHYS.P-141**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Thermodynamics and Kinetics of Multivalent Protein Interactions

Changeun Kim, Yongwon Jung[1], Jeong-Mo Choi[*]

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A multivalent interaction refers to an interaction between two molecules with multiple conjugate modules that can form multiple physical bonds. One can obtain stronger bonds from multiple weak monovalent interactions by using multivalent interactions. The intermolecular and intramolecular interactions determine the thermodynamics and kinetics of multivalent interactions. However, theoretical discussions have been mostly limited to the thermodynamic aspect, as the kinetics data were challenging to obtain experimentally. In this study, we studied the multivalent interactions between protein-binding partners, by observing the kinetics of association and dissociation through surface plasmon resonance (SPR). We developed a systematic method to extract the rate constants (k_{on} and k_{off}) from the noisy measurement data, and using the experimental data, we analyzed the nature of intermolecular and intramolecular interactions in several model systems. Particularly, we could separate the contributions of intramolecular and intermolecular interactions to the binding free energy, enthalpy, and entropy. A deeper understanding of the physicochemical basis of multivalent interactions will help us design and engineer biomolecular processes that involve multivalent interactions, such as biomolecular phase separation and drug design.

Poster Presentation : **PHYS.P-142**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of Charge Carrier-Selective Heterodyne Transient Grating Spectroscopic Technique and Its Application in the Distinction of the Surface Trap States in Hematite (α-Fe2O3)

Young Hyun Kim, Woon Yong Sohn*

Department of Chemistry, Chungbuk National University, Korea

We newly developed a spectroscopic technique which is named charge carrier-selective HD-TG (CS-HD-TG) method for the distinction of the surface trap states existing in the photocatalysts and photovoltaic materials by employing a burn laser inducing depletion of the number of the surface trapped charge carriers. In addition, as a case study, we measured HD-TG responses of hematite under bias condition with and without the burn laser and revealed that two distinct trap states co-exist at the surface in the hematite film and only one of them could act as the reaction intermediate for oxygen evolution reaction (OER), which is consistent with former studies.

Poster Presentation : **PHYS.P-143**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effects of Phase Separation on Protein Expression

Min Chung[*], **Jeong-Mo Choi**[1,*]

Department of Biomaterial Science and Department of Chemistry, Pusan National University, Korea
[1]*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 the noise in the protein concentration was greatly reduced when the protein was expressed asymmetrically (i.e., preferentially in either of the two phases), and that the noise reduction effect depended on the location of the phase boundary. 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.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Calculation of exciton couplings based on density functional tight-binding coupled to state-interaction state-averaged ensemble-referenced Kohn–Sham approach

Tae In Kim, **Seung Kyu Min***

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

Exciton diffusion is the transfer of electronic excitation from one chromophore to another within complex molecular systems such as photosynthetic systems, photovoltaic devices, and pigment-protein complexes. The electronic coupling between chromophores, termed excitonic coupling, plays a crucial role in determining the efficiency of exciton diffusion. Evaluating the excitonic couplings in molecular devices containing a numerous number of atoms requires high computational time. In this regard, the density functional based on tight binding (DFTB) method can be one of the promising candidates. In this study, we introduce a combination of the DFTB approach with onsite correction (OC) and long-range corrected (LC) functional and the state-interaction state-averaged spin-restricted ensemble-referenced Kohn–Sham (SI-SA-REKS or SSR) method with extended active space involving four electrons and four orbitals (LC-OC-DFTB/SSR(4,4)). We verify our method by evaluating locally excited (LE), charge transfer (CT) state, and excitonic couplings in anthracene/tetracene dimer and anthracene crystal with efficient computational cost.

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Poster Presentation : **PHYS.P-145**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

GPR based near-infrared D-luciferin analogue design using mutation accelerated graph-based genetic algorithm

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The discovery of molecules and their design has been a central aspect in the field of chemistry. In recent years, this field has become increasingly intertwined with data science such as machine learning (ML) and artificial intelligence (AI) methodologies. However, conventional molecular design methods such as neural network-based approaches require large databases, which can be inefficient in cases where the calculation cost for generating a target-specific database is large. Herein, we addressed this challenge of molecular design using a graph-based genetic algorithm (GB-GA), in which the mutation parameter is controlled to improve its optimization performance. For the accurate property prediction from a small database, we employed Gaussian processes regression (GPR) and utilized active learning strategies to construct a target-specific database. This algorithm was tested in the generation of near-IR luciferin for in-vivo bioimaging from an initial database of 187 luciferin analogue molecules. The results of this work suggest that this approach may be an appropriate method for designing molecules using a small database.

Poster Presentation : **PHYS.P-146**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Intramolecular Locking-Induced Heavy-Atom-Free Triplet-Utilizing Emitters with Aggregation-Induced Emission for Non-Doped OLEDs

Taehyun Kim, Dasol Chung, Taiho Park[*]

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

Efficient radiative decay properties and simple device structures are crucial characteristics of organic luminescent materials for potential optoelectronic applications. Therefore, heavy-atom-free triplet-utilizing emitters can act as next-generation luminogens with high internal quantum efficiency (IQE) and aggregation-induced emission (AIE) characteristics in a host-free non-doped system. Thereby, three asymmetric heavy-atom-free organic emitters were developed and their luminescent performance was investigated deeply. Intramolecular hydrogen bonding channel was formed in single crystal and detected in S-XRD measurement. Hydrogen bonding channel facilitate the intersystem crossing (ISC) rate and suppresses non-radiative deactivation resulting PLQY up to 94%. In addition, the hydrogen bonds produced intramolecularly locked crystal structures that form dense packed structure that detected in the two-dimensional grazing-incidence wide-angle X-ray diffraction (2D-GIWAXD). Interestingly, hydrogen bond triggered room temperature phosphorescence and AIE property were detected. It means that the compounds can applied to non-doped device structure. Consequently, a non-doped device was fabricated via vacuum deposition for OLED applications.

Poster Presentation : **PHYS.P-147**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Disclosing a Hidden Structural Origin of Two-Dimensional Colloidal Glasses with Machine Learning

Eun Cheol Kim, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Distinguishing glass states from liquid states based on structural information has been a challenging issue since the glass transition occurs without a notable structural change. Here, we present machine learning (ML) models based on convolutional neural network (CNN) to distinguish glasses from liquids using only structural information. Two-dimensional colloidal systems are a good proving ground due to the following reason: a large hexatic medium-range crystalline order (MRCO) appears in the configurations of two-dimensional polydisperse colloidal (2DPC) glasses but lacks in the configurations of binary glass counterparts (2DBC). We find that our ML models successfully classify the given configurations into glasses and liquids. This shows that one can determine the state of colloidal systems only with structural information. Furthermore, ML models trained with 2DBCs (where hexatic MRCO hardly appears in the glass states) also predict the glass transition of 2DPCs (where large hexatic MRCO appears in the glass states) well. This implies that the hexatic MRCO would not be the underlying structural origin of 2DPC glass transition.

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Poster Presentation : **PHYS.P-148**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The role of molecular oxygen(O_2) and UV light in the anion radical formation and stability of TCNQ and its fluorinated derivatives

Jieun Bang, **Jaehong Park**[1,*]

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

We report the electronic absorption spectroscopy of 7,7,8,8-tetracyanoquinodimethane (TCNQ) and its fluorinated derivatives (F_2TCNQ and F_4TCNQ), well-known electron-accepting molecules in common organic solvents (toluene, chlorobenzene, acetonitrile, and ethanol) under controlled exposure to air (O_2) and UV light. All compounds (F_xTCNQ(x = 0, 2, 4)) were stable in a neutral state (F_xTCNQ^0) in toluene and chlorobenzene, even under both O_2 and UV light. On the other hand, in EtOH, the formation of $F_xTCNQ^{\cdot-}$ was monitored upon controlled exposure to O_2 or UV light. Especially in air-equilibrated ethanol upon the UV-illumination, efficient α,α-dicyano-p-toluoylcyanide anion ($DCTC^-$) and its fluorinated derivatives were generated evinced by the absorption peak near 480 nm, whereas the reaction was shut off by removing O_2 or blocking UV light, thereby keeping $F_xTCNQ^{\cdot-}$ stable. However, even in deaerated ethanol, upon the UV-illumination, the anion formation of TCNQ and its fluorinated derivatives ($F_xTCNQ^{\cdot-}$, x = 0, 2, 4) was inevitable, showing the stability of F_xTCNQ^0 depends on the choice of solvent.

Poster Presentation : **PHYS.P-149**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Metastabilization in Phase Change Memory: A Crucial Role of Vacancies

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The reversible conversion between metavalent and covalent bonds, which can occur millions of times, has great potential as the basis for universal memory materials. To fully understand the crystal structures involved, studies on the kinetic behavior of vacancies are required. Although experimentally difficult, direct observation of vacancy behavior through density functional theory calculations has revealed that positively charged vacancies maintain the chemical state undisturbed. Also, the site-switching of vacancies in Sb2Te3 occurs gradually as the accumulation of vacancies triggers gliding along atomic planes to relieve electrostatic repulsion. The comprehension of the role of vacancies has been extended to the superlattices consisting of Sb2Te3 and GeTe sublayers that exhibit superior memory performance. The bandgap shift and charge redistribution show that the phase of the superlattice can be classified as metastable or stable, and that the conversion between metavalent and covalent bonds be achieved only in the metastable state.

Poster Presentation : **PHYS.P-150**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Surface and Interface Characteristics of Binary Self-Assembled Monolayers Formed by Coadsorption of Alkanethiols and N-heterocyclic Carbene Derivatives on Au(111)

Haeri Kim, Young Ji Son, Hyun Su Oh, Yeon O Kim, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) of organothiol molecules on metal substrates have been widely studied due to their practical applications in fields such as nanoscience, biosensors, and electronic devices. However, sulfur as a chemical anchor has low thermal and oxidative stability. N-heterocyclic carbenes (NHCs) have been proposed as an alternative having high chemical stability in solution or air than thiol. Mixed SAMs are known as a helpful method to control surface and interface properties in the nanoscale and are applied to various fields such as bio-interfaces and biosensors, electrical properties of molecular devices, and friction force control of surfaces. Binary mixed SAMs composed of two different compounds have been reported to exhibit properties that are distinct from those of the respective single-component monolayers. In this study, we synthesized 1,3-dimethyl-5-(octyloxy)-benzimidazolium hydrogen carbonate (C8-Me-NHC-HCO_3) to investigate the phase behaviors of NHCs and alkanethiols with different anchoring groups. We prepared binary mixed SAMs by coadsorption method in a 1 mM THF solution containing C8-Me-NHC and octanethiol as functions of molar ratios 10:90, 50:50, 90:10, 95:5 and 99:1 at 50 °C for 1 h. Subsequently, the prepared SAMs were thoroughly investigated by using scanning tunneling microscopy (STM), cyclic voltammetry (CV) and X-ray photoelectron spectroscopy (XPS).

Poster Presentation : **PHYS.P-151**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Improving the Efficiency of Quantum Chemical Computations through Atomic Orbital Space Segmentation

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Department of Chemistry, Yonsei University, Korea

In electronic structure calculations, there is always a trade-off between computational cost and accuracy depending on the system being computed. For large systems, some degree of accuracy must be sacrificed due to unaffordable computational costs. However, if the system is large enough, only some areas can be significantly affected when interacting with molecules. These regions are called active sites and have a greater influence on the interaction energy than the rest. The computational efficiency can be improved by concentrating on the active site. Embedding is a scheme that focuses on the active site and computes it at a high level, while the rest of the system, the environment, is computed at a lower level. By applying this, one can get the accuracy of higher-level calculations at the cost of lower-level ones. There are many methods for identifying the active site, but most methods have parameters such as the number of atoms in the active site that must be intuitively set for each system. In this work, we present a method to automatically distinguishing the active site through atomic orbital space segmentation, in which the energy of the system is divided for each atomic orbital to define the active site.

Poster Presentation : **PHYS.P-152**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Formation and Structure of 2,2'-Dipyrimidyl Disulfide Self-Assembled Monolayers on Au(111)

Dongjin Seo, Young Ji Son, Haeri Kim, Hyun Su Oh, Jun Hyeong Lee, 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. The binding energy of SAMs, significantly, can be changed by introducing a polar moiety in SAMs. A dipole moment can be introduced into the terminal group or alkyl chain of the molecules in the SAMs. Modifying the terminal group has a crucial shortcoming: dependency between binding energy and surface property. Embedding the dipole moment into the molecules of SAMs can solve the weakness of the terminal group modification method. Dipole moment can be embedded by introducing a pyrimidine ring into the alkyl chain. In this study, we studied the formation and structure of 2-mercaptopyrimidine SAMs, the simplest pyrimidine thiol, on Au (111) surface in various conditions by using its disulfide form, 2,2'-dipyrimidyl disulfide (2-DPyDS). We study the effects of immersion time, solvent, and concentration on the formation and structure of 2-DPyDS SAMs. To study the effects of molecule concentration and immersion time, we prepared 2-DPyDS SAMs immersed at RT in 0.1 mM, 0.01 mM, and 0.001 mM EtOH solutions for 2 h and in EtOH 0.01 mM solutions at RT for 30 min, 2 h, and 24 h. 2-DPyDS SAMs are also formed in THF, DMF, and EtOH 0.01 mM solutions at RT for 2 h, to study the effect of the solvents. The formation and surface structures of 2-DPyDS SAMs on Au(111) were examined using scanning tunneling microscopy, cyclic voltammetry, and X-ray photoelectron spectroscopy.

Poster Presentation : **PHYS.P-153**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular Self-Assembly of Alicyclic Thiocyanates on Au(111)

Jun Hyeong Lee, Young Ji Son, Haeri Kim, Hyun Su Oh, Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are commonly used to change surface properties since SAMs can be easily prepared and modified while changing targeted molecules. For two decades, many studies focused on Au(111) SAMs with thiol analogues but since thiols easily oxidize, changing headgroup to other compounds such as aliphatic thioacetates have been examined. Subsequently, Organic thiocyanates-based Au(111) SAMs are also studied because they are not easily oxidized and form well-ordered SAMs by cleavage of the S-CN bond. In this study, we fabricated cyclohexyl thiocyanate (CHTC) SAMs to form monolayers by breaking the S-CN bond in their headgroup instead of the S-H bond in thiols. After being synthesized with a simple S_N2 reaction, CHTC molecules are adsorbed on Au(111) in a 0.01 mM ethanol solution at room temperature. We also fabricated cyclohexane thiol SAMs with the same condition to compare with their thiol monologue. We characterized both SAMs through scanning tunneling microscopy (STM), cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS). With our STM-based surface analysis, we could observe a $(5 \times 2\sqrt{3})R30^\circ$ structure of both CHT and CHTC SAMs. We could observe more disordered phases and few vacancy islands on CHTC SAMs. CV-based reductive desorption shows that both SAMs possess almost the same peak around -1,000 mV and XPS measurements show that both SAMs have the same peak intensity when it comes to the S 2p, O 1s, and C 1s peak, while both SAMs never observed N 1s peak. Our data comparing CHT and CHTC SAMs demonstrated that CHTC molecules can be an excellent substituent when forming alicyclic SAMs.

Poster Presentation : **PHYS.P-154**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Formation and Structure of Self-Assembled Monolayers of N-heterocyclic Carbene Derivatives on Au(111)

Hyun Su Oh, Young Ji Son, Haeri Kim, Jun Hyeong Lee, Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are ultrathin films of organic molecules, usually composed of headgroup, backbone spacer, and terminal group. All the structural components play a crucial role in determining specific characteristics of the monolayers. The deposition of SAMs can easily modify the electrical and physical properties of solid surfaces. N-heterocyclic carbene (NHC) containing two nitrogen heteroatoms has been proposed as an excellent alternative to thiols forming SAMs because NHC-based SAMs on Au(111) have higher thermal/chemical stability than the typical thiol-based SAMs. In this study, we synthesized 1,3-diisopropyl-5-(dodecyloxy)-benzimidazolium hydrogen carbonate molecules to form SAMs on Au(111). We characterized the structural and electrochemical differences of the NHC SAMs using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV). We prepared single-component NHC SAMs using a solution deposition method in 0.1 mM and 1 mM THF solutions and an ethanol solution at 50 °C for 12 h, 24 h, and 48 h. Interestingly, NHC SAMs formed from low solution concentration exhibited a densely packed structure having higher stability. Our results will be helpful in the fundamental understanding of the structure and electrical properties of N-heterocyclic carbene SAMs.

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Poster Presentation : **PHYS.P-155**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Theoretical Elucidate of Li-ions Intercalation by Layer-Stacking Order at the Graphite Anode with Moment Tensor Potential

Jiwon Lee, Ji Seon Kim, Sang Uck Lee*

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In recent decades, many lithium-ion batteries (LIB) studies have been conducted to unveil the mechanisms of Li-ion transport and storage that occurred at anodes. Although it is well known that Li-ions (de)intercalates as stage reactions, it is still not clear to finely explain. According to previous studies, Li-ions fully inserted between the vertically arranged graphite layers is (de)interclated one layer during the charging/discharging process of LIB. Based on the above points, we systemically carried out a simulation to investigate Li ions pathway. In our study, we designed a lot of Li-graphite layer structures with various ratios of Li/C based on cluster expansion theory to demonstrate a theoretical view of the Li-ions (de)intercalations. To overcome the high computational costs induced by the number of DFT simulation cases, we adjusted moment tensor potential (MTP), one of the machine-learning interatomic potentials based on the DFT results. Then, we efficiently obtained the most stable structures for each ratio using MTP. Notably, unlikely the known result, our simulations propose a new perspective on the Li-ion arrangement of Li when deintercalated. Based on these theoretical results, our finds would allow an in-depth understanding the Li pathway, and contribute to the electrode material designing and optimizing rechargeable LIB.

Poster Presentation : **PHYS.P-156**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Bioinformatic Analysis of Protein Structures Using Contact Map Formalism

TaeHwan Kim, Jeong-Mo Choi*

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Structural information of a protein is the key to understanding its function. Various experimental methods such as X-ray crystallography, NMR spectroscopy, and cryo-EM have been developed to determine the structures of proteins, and efforts are still being made to predict biomolecular functions by analyzing the structural information. It has been shown that topological information of a protein structure is often sufficient to extract the principles of protein folding and design. Here, we represent the protein structures by contact maps; a contact map (CM) is a 2-dimensional matrix that contains information about the contacts between residues in a protein. We tested several quantities (such as trace and element sum) derived from a CM to characterize a protein structure, and found that CMs can reveal structural and evolutionary diversity of proteins.

Poster Presentation : **PHYS.P-157**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

D-glucosamine-conjugated PAA-coated ultrasmall gadolinium oxide nanoparticles in MRI and cancer imaging

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Lanthanide oxide nanoparticles have attracted extensive attention in biomedical imaging field owing to its exclusive advantages such as good mechanical stability, high surface area and paramagnetic properties. In particular, because their paramagnetic moments at room temperature are sufficiently high to induce water proton spin relaxations, lanthanide oxide nanoparticles play an important role in magnetic resonance imaging (MRI), drug delivery and tumor targeting. Owing to a higher demand for glucosamine (GlcN) in metabolic processes in cancer cells than in normal cells (i.e., GlcN effects), cancer imaging in magnetic resonance imaging (MRI) can be highly improved using GlcN-conjugated MRI contrast agents. Here, GlcN was conjugated with polyacrylic acid (PAA)-coated ultrasmall gadolinium oxide nanoparticles (UGONs) (d_{avg} = 1.76 nm). Higher positive (brighter or T_1) contrast enhancements at various organs including cancer were observed in human brain glioma (U87MG) tumor-bearing mice after the intravenous injection of GlcN-PAA-UGONs into their tail vein.

Poster Presentation : **PHYS.P-158**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tumor-targeting Ligand Conjugated to Poly (acrylic acid)-Coated Gadolinium Oxide Nanoparticles for Enhanced Tumor Imaging

Mohammad Yaseen Ahmad, Gang Ho Lee[1,*]

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In this study, Biotin (Bio) as a tumor-targeting ligand, conjugated poly(acrylic acid) (PAA), and coated gadolinium oxide (Gd_2O_3) nanoparticles (Bio-PAA-Gd_2O_3 NPs) were synthesized by a polyol method, and physiochemical properties of the nanoparticles were investigated using various techniques. The nanoparticles exhibited a high relaxation (r^{-1}) value of 23.8 $s^{-1}mM^{-1}$ (r_2 /r_1 = 1.6, r_2 = transverse water proton spin relaxation), which is about 6 times higher than the r_1 value of commercial molecular contrast agents. The results of toxicity on HepG2 tumor cell (human liver cancer cell line) and HEK-293 normal cell (immortalised cell line) showed that Bio-PAA-Gd_2O_3 NPs sample had non-toxic up to 500 μMGd both cell lines. In vivo T_1 -MRI showed positive (or T_1) enhanced contrast in tumor-bearing liver and kidney compared to controls after intravenous administration including tumor, indicating that Bio-PAA-Gd_2O_3 NPs act as enhanced cancer imaging agents similar to tumor targeting agents in T_1 MRI. The heart, lung, liver, aorta, and kidney were among the other cancer sites that were evaluated. According to in vivo studies, the accumulation of nanoparticles in tumors was considerably boosted by tumor-targeting ligands.

Poster Presentation : **PHYS.P-159**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Gadolinium oxide nanoparticles coated by carbon for MRI and FI dual-modal imaging

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The molecular imaging is an extremely important technique in diagnosing diseases field. Dual imaging can provide us with more information for diagnosing disease than single imaging. The nanomaterials combined with magnetic resonance imaging (MRI) and fluorescent imaging (FI) mode is a promising tool. Herein, a novel kind of carbon coated ultrasmall gadolinium oxide (Gd_2O_3@C) nanoparticle with diameter of 3.1±1.0 nm was obtained by a facile method for MRI and FI. The obtained Gd_2O_3@C NP exhibited not only high longitudinal relaxivity (r_1=16.26 s^{-1} mM^{-1}) but also excellent colloidal stability. Meanwhile, the nanoparticles showed a strong fluorescence in the visible region and fluorescence confocal images on a micrometer scale due to carbon coating. Therefore, the ultrasmall Gd_2O_3@C NPs can be severed as promising MRI and FI dual modal contrast agent to provide more accurate and comprehensive diagnosis information.

Poster Presentation : **PHYS.P-160**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ultrasmall Holmium Oxide Nanoparticles Coated by Polyethylenimine as T_2 MRI Contrast Agents

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The polymers or ligands used for surface coating could greatly influence the colloidal stability, biocompatibility and relaxivities of the magnetic resonance imaging (MRI) contrast agents. Polyethylenimines (PEIs) of two different molecular weights (Mn = 1200 and 60,000 amu) were chosen as surface-coating ligands of holmium oxide (Ho_2O_3) in this work. The ultrasmall average particle diameter of 2.0 and 1.9 nm for the obtained PEI1200- and PEI60000-coated ultrasmall Ho_2O_3 nanoparticles, respectively, could achieve excellent stability, low cytotoxicity and negligible longitudinal relaxivities (r_1) and appreciable transverse relaxivities (r_2) of 13.1 and 9.9 $s^{-1}mM^{-1}$ in 3.0 T MR filed. Therefore, the R_1 and R_2 map images of both samples show the negligible r_1 and the dose-dependent r_2, respectively, which allows both samples possess the potential efficient T_2 MRI contrast agents.

Poster Presentation : **PHYS.P-161**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis, Characterization, And Cytotoxicity of Polyacrylic Acid Coated Gadolinium Oxide Nanoparticles as High-Performance T_1 Magnetic Resonance

Abdullah Al saidi, Gang Ho Lee[1,*]

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Ultrasmall Gd_2O_3 nanoparticles can potentially be used as a positive magnetic resonance imaging (MRI) contrast agent owing to their high content of Gd (III), which exhibits the highest spin magnetic moment of all elements due to its seven unpaired 4f electrons. Gadolinium oxide nanoparticles should be stable, non-toxic, and ultrasmall in particle diameter for renal excretion, and need to be coated with hydrophilic biocompatible ligands. In addition, they should have a high longitudinal water proton relaxivity (r_1) and r_2/r_1 ratio that is close to one (r_2 = transverse water proton relaxivity) for high performance. In this study, we report ultrasmall Gd_2O_3 nanoparticle colloids were coated with hydrophilic biocompatible polyacrylic acids (PAA, M_w = ~ 5100 Da) satisfying these conditions. The particle diameter was monodisperse with an average value of 2.0 nm. The colloidal suspension exhibited a high r_1 value of 31.0 s^{-1} mM^{-1} and r_2/r_1 ratio of 1.2, where r_1 was ~ 8 times higher than that of commercial Gd-chelates: the cooperative induction model was proposed to explain this. The effectiveness of the colloidal suspension as a high-performance T_1 MRI-CA was confirmed by taking in vivo T_1 MR images in a mouse after intravenous administration. Highly positive contrast enhancements were observed in various organs of the mouse such as the liver, kidneys, and bladder. The colloidal suspension was then excreted through the bladder.

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Poster Presentation : **PHYS.P-162**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation and characterization of monodisperse magnetic iron oxide nanoparticles

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Because of their unique magnetic properties, nontoxicity, and biodegradability, superparamagnetic iron oxide nanoparticles have been increasingly employed for biomedical applications. In this study, we report nearly monodisperse Fe_3O_4 and $Fe@Fe_3O_4$ (core: Fe, shell: Fe_3O_4) nanoparticles in aqueous phase under argon flow, and coated them with various biocompatible ligands and silica. We characterized the prepared surface-modified nanoparticles using HRTEM, XRD, FT-IR, SQUID, PL, and Confocal microscopy.

Poster Presentation : **PHYS.P-163**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Density-Corrected DFT for Large Systems

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Density-corrected density functional theory (DC-DFT) is a theoretical framework for identifying failures in density functional approximations by separating errors of the approximated functional itself from errors due to its self-consistent density. For some systems, Hartree-Fock density is known to reduce density-driven errors. In that case, DC(HF)-DFT is one of the practical DC-DFT methods. Recently, it has been reported that HF-r2SCAN-DC4, based on DC-DFT principle, works particularly well in water-containing systems, making it suitable for aqueous solution simulations and relevent chemical reactions. Hartree-Fock perturbative correction (HFPC) is a method of improving the Hartree-Fock calculation towards the complete-basis limit with a much lower computational cost. In this work, we discuss the performance of DC(HFPC)-DFT for large systems with respect to accuracy and computational cost.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An uncertainty-aware machine learning algorithm based on graph convolutional network and linear regression

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Machine learning (ML) models are widely applied to predict properties of materials and molecules. In these applications, graph neural network (GNN) methods show remarkable performance. When GNNs are trained for molecular datasets, molecular features are extracted from molecular structures, usually given in SMILES or 3D coordinates, through graph convolutional layers. Then, target properties can be predicted by introducing molecular features into fully connected layers. In this work, we present an ML algorithm that can predict both molecular properties and its prediction uncertainties using the fact that graph convolutional layers can provide enough information about molecular features. For this purpose, after training the graph convolutional network (GCN), we replaced the time-consuming fully connected layers to a linear regressor. We found that this modification does not change the performance of ML models. We are able to show that our new algorithm can be used to quantify prediction uncertainty. We expect this method to be a practical method for estimating both molecular properties and their prediction uncertainties at the same time.

Poster Presentation : **PHYS.P-165**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Excited-state charge transfer and proton transfer dynamics by impulsive stimulated Raman spectroscopy

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Time-resolved Raman spectroscopy has been widely employed to investigate ultrafast structural changes of chromophores during the charge transfer and proton transfer processes in the excited states. Recently, the skeletal vibrational modes of ν_{8a} and $\nu_{C=C}$ in 1500-1650 cm^{-1} have been reported to be sensitive to the structural changes of the π-conjugated backbones (styrylpyran, biphenyl, and stilbene) of several push-pull chromophores accompanying the excited-state intramolecular charge transfers (ICTs) by femtosecond stimulated Raman spectroscopy (FSRS). Moreover, the strong coherent oscillations have been observed in most of the skeletal vibrations of 4-dimethylamino-4'-nitrostilbene, which shows that the charge transfer reaction coordinate may be anharmonically coupled to the low-frequency vibrational modes (80-155 cm^{-1}) possibly leading to the twist of the nitrophenyl group during the ICT. In this work, the low-frequency vibrational modes ($^{-1}$) of chromophores will be directly monitored by impulsive stimulated Raman spectroscopy (ISRS) based on the broadband (>60 nm,

Poster Presentation : **PHYS.P-166**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Miniature Reflectron Time-of-Flight Mass Spectrometer for in situ Monitoring of Process Control

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The mass spectrometer is one of the most powerful instruments for analyzing a broad spectrum of chemical and biological materials, but its applicability to field detection problems has been limited given its large size and heavy weight. In this work, we describe the development of a miniature reflectron time-of-flight (TOF) mass spectrometer, based upon a diverging, annular TOF 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. 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-167**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Highly Sensitive Near-Infrared SERS Nanoprobes for In Vivo Imaging using Gold-Assembled Silica Nanoparticles with Controllable Nanogaps

Yun sik Choi, Dae Hong Jeong, Hyejin Chang[1,*]

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[1]*Division of science education, Kangwon National University, Korea*

To take advantages, such as multiplex capacity, non-photobleaching property, and high sensitivity, of surface-enhanced Raman scattering (SERS)-based in vivo imaging, development of highly enhanced SERS nanoprobes in near-infrared (NIR) region is needed. A well-controlled morphology and biocompatibility are essential features of NIR SERS nanoprobes. Gold (Au)-assembled nanostructures with controllable nanogaps with highly enhanced SERS signals within multiple hotspots could be a breakthrough.Au-assembled silica (SiO2) nanoparticles (NPs) (SiO2@Au@Au NPs) as NIR SERS nanoprobes are synthesized using the seed-mediated growth method. SiO2@Au@Au NPs using six different sizes of Au NPs (SiO2@Au@Au50–SiO2@Au@Au500) were prepared by controlling the concentration of Au precursor in the growth step. The nanogaps between Au NPs on the SiO2 surface could be controlled from 4.16 to 0.98 nm by adjusting the concentration of Au precursor (hence increasing Au NP sizes), which resulted in the formation of effective SERS hotspots. SiO2@Au@Au500 NPs with a 0.98-nm gap showed a high SERS enhancement factor of approximately 3.8 × 10^6 under 785-nm photoexcitation. SiO2@Au@Au500 nanoprobes showed detectable in vivo SERS signals at a concentration of 16 µg/mL in animal tissue specimen at a depth of 7 mm. SiO2@Au@Au500 NPs with 14 different Raman label compounds exhibited distinct SERS signals upon subcutaneous injection into nude mice. SiO2@Au@Au NPs showed high potential for in vivo applications as multiplex nanoprobes with high SERS sensitivity in the NIR region.

Poster Presentation : **PHYS.P-168**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Dual Filament Assembly in a Linear Time-of-Flight Mass Spectrometry

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A miniature linear time-of-flight mass spectrometer (TOFMS) with electron impact (EI) ionization source has been reported in the 128th General Meeting of the Korean Chemical Society to perform in situ gas composition analysis in a process monitoring. The upper limit of the mass range is greater than 500 amu, and the best resolving power obtained so far on the miniature TOFMS is around 200 at full width half maximum (FWHM). In this work, feasibility of a dual filament assembly was evaluated by monitoring the N_2 and O_2 ion signal originated from ambient air. The results indicate that this compact filament assembly provides extended operation and lifetime. In addition, the sustainability of the W wire is compared with that of the Re and W-Re alloy.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Detection of cancer cells using SERS with Fe_2O_3@SiO_2@Au nanoparticles

Hae-jin Chung, Eungyeong Park, Shuang Guo, Young Mee Jung*

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Circulating tumor cells (CTC) separate from the tumor and then spread in the blood, causing new disease. CTC detection as a liquid biopsy of tumors can be used for early diagnosis. Surface-enhanced Raman scattering (SERS) with ultra-sensitivity, selectivity, and photostability is introduced for easier CTC detection methods than biopsy. In this study, Fe_2O_3@SiO_2@Au nanoparticles (Fe_2O_3@SiO_2@Au NPs) were fabricated for SERS detection of CTC. Since Fe_2O_3 is a magnetic core, Fe_2O_3@SiO_2@Au NPs can easily separate cancer cells from a complex system. The properties of Fe_2O_3@SiO_2@Au NPs were investigated by transmission electron microscope, energy-dispersive X-ray spectroscopy, UV-Vis absorption spectroscopy, and SERS. Details on SERS spectra of CTC will be explained in the presentation.

Poster Presentation : **PHYS.P-170**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The impact of oligothiophene linkers in triplet formation pathways of 6,6’-linked pentacene dimers

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Singlet Fission (SF) is a process that generates two triplet excitons from one singlet exciton, and it occurs uniquely in organic semiconducting materials.[1] This phenomenon has attracted considerable attention because it has the potential to surpass the Shockley-Queisser limit owing to carrier multiplication in photovoltaics.[2,3] To produce two excitons, it is necessary to have at least two closely interacting chromophores, making a covalently linked molecular dimer the simplest model for understanding the SF mechanism.[4] In this study, we investigated the intramolecular SF dynamics of 6,6'-linked pentacene dimers with various types of oligothiophene linkers to understand their roles in manipulating SF pathways. Through analysis of femtosecond transient absorption (TA) spectra, we discovered that the spectral evolution behaviors and kinetics varied significantly depending on the number of oligothiophenes and the presence of ring fusion. Moreover, we observed the impact of conformational heterogeneity by selectively exciting specific conformers with red-edge excitation. Overall, we believe that our study can provide molecular design rules for efficient intramolecular singlet fission.References [1] Smith, M. B.; Michl, J. Singlet Fission. Chem. Rev, 2010, 110, 6891−6936.[2] Shockley, W.; Queisser, H. J. Detailed Balance Limit of Efficiency of p-n Junction Solar Cells. J. Appl. Phys, 1961, 32, 510– 519.[3] Hanna, M. C.; Nozik, A. J., Solar conversion efficiency of photovoltaic and photoelectrolysis cells with carrier multiplication absorbers. J. Appl. Phys, 2006, 100, 074510.[4] Korovina, N. V.; Pompetti, N. F.; Johnson, J. C. Lessons from Intramolecular Singlet Fission with Covalently Bound Chromophores. J. Chem. Phys. 2020, 152 (4), 040904.

Poster Presentation : **PHYS.P-171**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular Dynamics Energetics of Amyloid Fibril Polymorphs

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

Amyloid fibrils are molecular hallmarks of neurodegenerative diseases, such as Alzheimer’s disease, Parkinson’s disease, and type Ⅱ diabetes. The same protein can have different structures when forming amyloid fibrils, which is known as polymorphism. Although the full relationship of amyloid fibrils to the diseases has not been revealed, it was suggested that fibril stability is correlated with pathological risk. In this work, we have used standard molecular dynamics simulations combined with umbrella sampling to analyze the thermodynamics of amyloid beta (Aβ) polymorphs. We could successfully decompose energetic and entropic contributions to monomer binding affinity and revealed the full thermodynamics of Aβ fibrillation.

Poster Presentation : **PHYS.P-172**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Study of chitosan-based hydrogels for drug delivery

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Hydrogels have properties similar to biological tissue, and are thus widely used in numerous applications so far. Here we synthesized photo-reversable hydrogels based on reversibly photo-controllable association/dissociation behavior of Dropna145N, a tetrameric green fluorescent protein. Chitosan, a natural polymer, was modified to be conjugated with maleimide moiety. Maleimide and -SH group of cysteine at 113 form covalent bond to make cross-link networks of the hydrogels. These hydrogels underwent reversible sol-gel transition due to photo-dissociation/association of Dronpa 145N by cyan and violet light. It also showed reversible on-off behavior of green fluorescence upon the same light illumination. The photo-controllable gel-sol transition can be used to a drug delivery system for the light-controlled release of the small molecules.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

In Silico Engineering of Binding Affinities of Green Fluorescent Proteins

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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-174**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Characteristics of photo-reversible hydrogels synthesized from Chitosan and pdDronpa

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Hydrogel is a soft material that has higher water content inside its mesh-like structure. Externally controllable hydrogels have received a lot of attention due to its wide applicability. pdDronpa is a dimeric green fluorescent protein which is a derivative of tetrameric Dronpa 145N. It has a faster light conversion rate than Dronpa 145N and forms less aggregates, making it suitable for photo-reversible hydrogel synthesis. Hydrogel were synthesized from pdDronpa, linear dithiol polyethylene glycol (PEG), and chitosan maleimide. Thiol group at 113 position of pdDronpa reacted with maleimide to form a covalent bond that is a key reaction for cross-link. Synthesized hydrogels underwent reversible sol-gel transition under illumination of cyan and violet light. Spatiotemporally tuning of hydrogel is considered to be applicable to drug delivery system.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Adsorption and bulk diffusion of hydrogen on Pd nanowires.

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

Palladium has attracted a significant amount of attraction because of its potential application as a catalyst, energy storage material, gas sensor and other electronic devices. Sorption of hydrogen into Pd is an important research topic to understand the chemical and physical properties of Pd. We have fabricated Pd nanowires with different diameters using anodized aluminum oxide (AAO) templates to study the diffusion of hydrogen into the bulk of Pd. We will report the adsorption and bulk diffusion of hydrogen on pd nanowires in the gas phase and aqueous solutions.

Poster Presentation : **PHYS.P-176**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mass correlated rotational Raman spectrum and fragmentation of CS_2 monomer and dimer.

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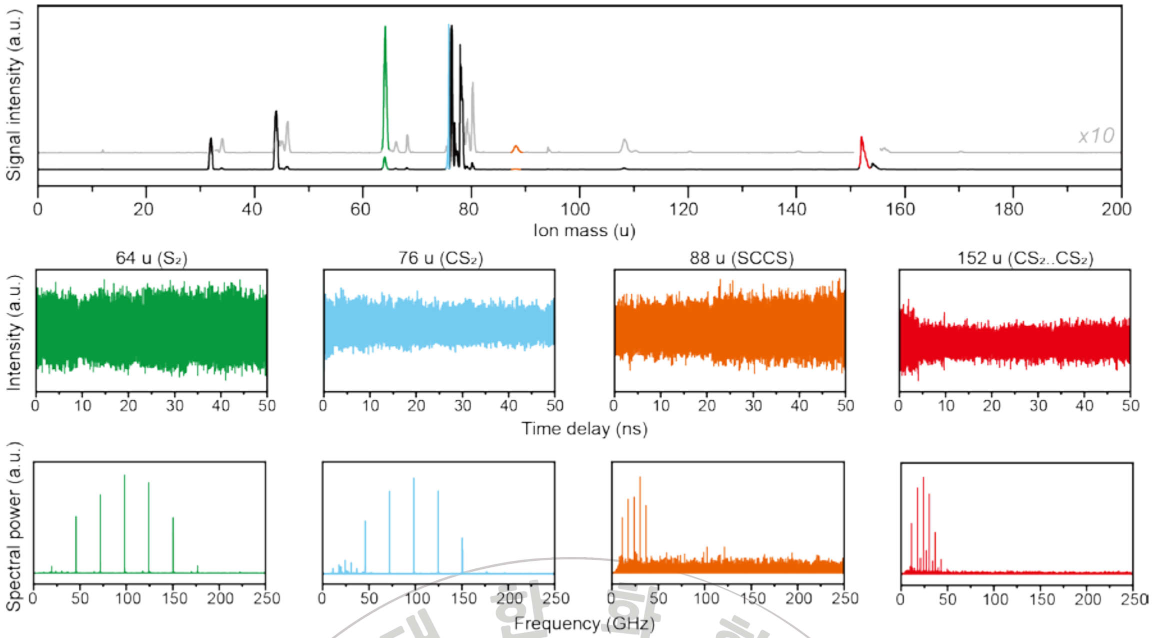
Molecular photodissociation plays an important role in astrophysical, biological and chemical environments. To characterize photochemical reaction mechanisms, we need to first characterize the structure and properties of the parent molecules before fragmentation and, second, characterize the structure and properties of formed fragments. Past experimental investigations typically skipped the first step, which is only possible if the reacting sample is homogeneous and well-characterized. Mass-correlated rotational alignment spectroscopy (CRASY) observes molecular fragments in a mass spectrometer and correlates each fragment mass with the rotational Raman spectrum of the parent molecule. The mass correlated rotational Raman spectra reveal the origin of fragments even in impure, heterogeneous samples. CRASY, therefore, can characterize photodissociation pathways in heterogeneous samples, where past investigations failed or had to resort to speculative interrpretation. In this poster, we present a mass-CRASY experiment with a CS_2-cluster sample and resolve the rotational Raman spectrum of the molecular isotopologues, the moelcualr dimer, and a wealth of molecular fragment. The result shows that signals in the mass channel 64 u (S_2), 76 u (CS_2), and 88 u (SCCS) are formed from the CS_2 dimer parent molecule. The corresponding fragmentation channels are further analyzed by ab initio calculations.


Signal intensity (a.u.)
x10
0
20
40
60
80
100
120
140
160
180
200
Ion mass (u)
64 u (S₂)
76 u (CS₂)
88 u (SCCS)
152 u (CS₂..CS₂)
Intensity (a.u.)
0
10
20
30
40
50
Time delay (ns)
Spectral power (a.u.)
0
50
100
150
200
250
Frequency (GHz)

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Poster Presentation : **PHYS.P-177**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Improving electrochemical hydrogen production using non-metal-doped transition metal carbide (TMCs) catalysts

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

Hydrogen energy is attracting attention worldwide due to recent industrial and environmental changes because hydrogen energy is not affected by local conditions, unlike solar, wind, and geothermal energy. In particular, green hydrogen, produced by decomposing water into hydrogen and oxygen, is attracting attention. Since the catalyst determines the efficiency and cost of hydrogen production, the catalyst is a crucial factor. This study developed a low-cost, high-efficiency catalyst for hydrogen production by doping transition metal carbide with a non-metal. Nitrogen-doped molybdenum carbide was synthesized using a pulsed laser system. As a result, the crystal structure (MoC, Mo_2C) of molybdenum carbide was confirmed using XRD. The morphology and constituent elements were confirmed using SEM and EDS. Finally, it was confirmed by Raman and XPS that nitrogen was doped into molybdenum carbide. Finally the catalyst optimized for hydrogen production through physical property analysis was analyzed through HER and OER analysis. The nitrogen-doped molybdenum carbide developed through this research is expected to be used as an inexpensive and highly efficient catalyst for green hydrogen production in the future.

Poster Presentation : **PHYS.P-178**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

In-situ growth of CoO and Cu_2O on nickel foam via pulsed laser irradiation for furfural oxidation reaction

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Replacing kinetically sluggish oxygen evolution reaction (OER) by organic molecule oxidation reaction emerging as it enables efficient H_2 fuel and high-value-added production. Transition metal oxides (TMOs) attracted much attention as an alternative of noble metal-based electrocatalysts because of the earth-abundant and high oxidation nature of TMOs resulting in enhanced catalytic activity. Herein, we successfully fabricated TMOs such as CoO and Cu_2O on nickel foam via pulsed laser irradiation technique in an aqueous medium. This method demonstrates a time saving and simple way to fabricate enhanced binder-free electrode which provides high electron conductivity. The synthesized materials were characterized by XRD, Raman, FE-SEM, and XPS analytical techniques, and employed as an electrocatalysts for oxygen evolution reaction (OER) and furfural oxidation reaction (FOR), respectively. Among the fabricated electrodes, CoO/Ni foam exhibited a highest OER as well as FOR performances. This study provides facile way of fabrication electrodes which can be utilized for the multi-functional electrocatalytic reaction towards the production of energy-saving H_2 fuel and 2-furoic acid as value-added products.

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Poster Presentation : **PHYS.P-179**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile synthesis of Co-loaded reduced graphene oxides via pulsed laser for electrochemical oxygen evolution reaction

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Recently, pulsed laser assisted synthetic strategies have been considered as one of the facile methods for the development of efficient electrocatalytic nanomaterials. Cobalt containing reduced graphene oxide (Co-rGO) hybrids were synthesized via single-step pulsed laser irradiation in which the uniform Co nanoparticles were attached in thin layers of rGO nanosheets. Initially, graphene oxide was reduced to rGO using ascorbic acid, a weak reducing agent via pulsed laser. Thus, the synthesized rGO and Co-rGO materials were 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. The electrochemical properties of the Co-rGO towards oxygen evolution reaction in alkaline medium were examined and investigated the effect of Co loading in the efficiency of oxygen evolution. The obtained results suggest that the Co-rGO nanocomposite is a promising material for electrochemical energy production applications.

Poster Presentation : **PHYS.P-180**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Real-time Study of Methylene Blue Dimerization using an Acoustic Levitator: A Spectroscopic and DFT study

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The acoustic levitator is a novel and unique technique that enables containerless processing of a single free-standing droplet. The support-free levitator droplet act as a reactor in the air medium. It can avoid several complex effects at the contact surfaces of materials, such as reaction vessels, and increase the sensitivity of spectral detection techniques such as Raman spectroscopy, Ultraviolet-Visible (UV-Vis) spectroscopy, Fourier-transform infrared spectroscopy, and Intensified charge-coupled device (ICCD) camera. Herein, we studied the dimerization of methylene blue using various solvents (organic and aqueous) via acoustic levitator. The dimerization of methylene blue is greatly affected by the dielectric constant of the solvent medium. We observed real-time reactions by altering the composition of solvents, which directly influence the dimerization of methylene blue. Besides water droplet, the UV-visible spectrum shows the changes in the resolved two peaks when methanol and ethanol was used as solvent. Interestingly, we could observe the dimerization phenomenon in methanol and ethanol solvents due to the evaporation of droplet, which could be difficult to observe in the container reaction due to its low dielectric constant compared to water medium. Moreover, acidic protonation shows a change in the direction of aggregation of the MB molecules. These results were further confirmed through DFT calculations.

Poster Presentation : **PHYS.P-181**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Metal-organic frameworks derived $RuCoO_x$@nitrogen-doped carbon composite as an efficient electrocatalyst for hydrazine-assisted energy-saving hydrogen production

Senthil Raja Arumugam, Sieon Jung, Seung Jun Lee[1], Myong Yong Choi*

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Hydrogen has been recognized as a suitable carbon-free energy resource to replace traditional fossil fuels. Water electrolysis is one of the most promising technologies to generate clean hydrogen energy from the splitting of water molecules. However, its widespread application is restricted from the sluggish anodic oxygen evolution reaction (OER). Therefore, the coupling of the hydrogen evolution reaction (HER) with low-potential hydrazine oxidation reaction (HzOR) is extremely capable to decrease the input cell voltage of water electrolysis. Herein, a report a facile approach to developing the $RuCoO_x$@nitrogen-doped carbon ($RuCoO_x$@NC) composite from metal-organic frameworks (MOFs) as a metal precursor and self-template for the hydrazine-assisted energy-saving hydrogen production in alkaline media. The as-synthesized $RuCoO_x$@NC composite exhibited the excellent HER and HzOR performance with low overpotential of 44 and 290 mV at 10 mA cm^{-2}, respectively. Moreover, the fabricated overall hydrazine splitting electrolyzer with $RuCoO_x$@NC composite as both anode and cathode needed an ultra-low cell voltage of only 0.063 and 0.505 V to produce 10 and 50 mA cm^{-2}, respectively with an amazing long-term stability for 12 h. This work offers a promising electrocatalytic material for the energy-saving hydrogen production.

Poster Presentation : **PHYS.P-182**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigation of Exciplex between Poly Aromatic Hydrocarbons and *N*,*N*-dimethylaniline: Efficiency of Exciplex Formation and their Radiative Decay

Ena Yun, Hohjai Lee[*]

Chemistry, Gwangju Institute of Science and Technology, Korea

Exciplex (Xplx) is an emissive complex, formed through charge transfer from a ground state donor (D) to photon-excited acceptor (A*). Due to its radiative properties, Xplx has been extensively studied for photo-induced electron transfer (PET) mechanism and the development of Xplx-based organic light-emitting diode (OLED). In this work, we tried to investigate the Xplx-forming efficiency between A/D pairs and Xplx emissivity. Polycyclic aromatic hydrocarbons (PAHs), such as anthracene, tetracene, pyrene, perylene, and *N*,*N*-dimethylaniline (DMA) was selected as A and D, respectively, since they are well-known Xplx-forming A/D pairs. To discuss the Xplx formation process, thermodynamic driving force of PET and quenching rate constants (k_q) of each A* by D were experimentally determined. To describe its emissivity of each A/D pair, we designed the Xplx kinetic model based on measured the quantum yield of Xplx emission and its decay time. Also, we performed quantum-chemical calculations and simulated their emission spectrum using density functional theory (DFT) and time-dependent DFT (TD-DFT) to obtain more details about Xplx geometry and orbital overlap between A/D. The results suggest that the larger energy gap between high occupied molecular orbital (HOMO) of A/D result in the greater contribution of D for Xplx HOMO. To describe the Xplx states, the orbital overlap between A/D, oscillator strength of Xplx and charge transfer index should be considered. This study will provide details about the radiative decay properties of Xplx formed between various PAHs and DMA.Acknowledgements This work was supported by Samsung Science & Technology Foundation under Project Number SSTF-BA2002-10.

Poster Presentation : **PHYS.P-183**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Rational design of flower like Co-CuO by pulsed laser ablation as robust electrocatalyst for methanol oxidation with energy-saving hydrogen production

Sieon Jung, Senthil Raja Arumugam[1], Seung Jun Lee[2], Myong Yong Choi[1,*]

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Electrochemical water splitting is one of the most ideal ways to produce hydrogen energy to replace fossil fuels. However, the large-scale hydrogen production is seriously suffered from the sluggish kinetics of anodic oxygen evolution reaction (OER). The electrochemical methanol oxidation reaction (MOR) coupled with hydrogen evolution reaction (HER) is considered as an innovative approach to achieve energy-saving co-generation hydrogen and value-added chemicals. Herein, we reported a flower like Co doped CuO (Co-CuO) nanostructures via an advanced pulsed laser ablation (PLA) strategy and used as an electrocatalyst for MOR in alkaline media. The electrochemical results show that Co-CuO exhibited a superior MOR performance as compared with pristine CuO, which is demonstrating that the synergistic effect of Co-doping. Furthermore, Co-CuO electrocatalyst showed a lower potential of 1.51 V @ 10 mA cm^{-2} toward MOR when compared to its OER performance (1.68 V @ 10 mA cm^{-2}). Through coupling of HER on the cathode and MOR on the anode, the efficient hydrogen production was achieved with generation of value-added chemicals. This work provides a novel strategy for the rational design of nanomaterials with efficient electrocatalytic performance.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

High-entropy oxides on 2D MXene nanosheets with V, Mn, Co, Ni, and Fe via microwave-heating with oxygen evolution performance

Chae Eun Park, Gyoung Hwa Jeong[1], Myong Yong Choi[*]

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[1]*Gyeongsang National University, Korea*

High entropy oxides (HEO) is a new type of single-phase solid solution material. Transition metal-based HEO has recently attracted increasing interest as a potential positive electrode for energy storage and conversion materials due to its high storage capacity and cycle reversibility. In this study, MXene@(V, Mn, Fe, Co, and Ni) HEO was synthesized by using two methods like microwave and CO_2 laser. Microwave has the advantage of high-performance wavelengths with good absorption bandwidth and low density. CO_2 laser can synthesize materials by irradiating high power with thermal energy rather than light energy. Our synthesized HEO materials' characterizations were investigated from SEM, TEM, XRD, XPS and ICP measurements. In addition, the electrochemical test on the oxygen evolution was performed to measure their catalytic activities.

Poster Presentation : **PHYS.P-185**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Pulsed laser synthesis of hierarchical noble-metal-doped nickel phosphate as an efficient bifunctional catalyst for electrochemical water splitting

Hyeyeon Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Water electrolysis is the most promising environment-friendly approach for generating hydrogen on a large scale with the highest efficiency and purity. It is governed by hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) processes, but the sluggish OER is more decisive and rate-determining. The most recent oxygen- and hydrogen evolving electrocatalysts with the highest performance are noble metal-based catalysts (i.e., Pt, Ru and Ir). However, these metals are finite in the earth crust, which limits their wide application. Therefore, extensively studied transition metal-based electrocatalysts could be alternatives to expensive noble metals in the HER and OER. Phosphate, as a new series of electrocatalysts, has attracted enormous attentions, owing to its unique lattice structure geometry. The phosphate group not only benefits the adsorption of water molecule but also facilitates the oxyhydrate of metal site and dissociation of water. In this work, we produce $Ni_2(PO_4)_2{\cdot}8H_2O$ electrocatalysts via pulsed laser irradiation in liquid (PLIL) and explored the phase-selective active-sites in electrocatalytic HER and OER, respectively. Further, the various noble-metal such as Pt, Pd, and Ru nanoparticles was incorporated by PLIL process to enhance the active sites of $Ni_2(PO_4)_2{\cdot}8H_2O$ catalysts. The synthesized catalysts were characterized using various analytical techniques such as XRD, FE-SEM, EDS, and XPS. This work not only shows PLAL-synthesized electrocatalysts as promising candidates for water splitting, but also provides an underlying principle for advanced energy-conversion catalysts and beyond.

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Formation Mechanism of Alkali Halide Cluster Ion During the Electrospray Ionization

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

There are many studies to demonstrate the mechanism of ionic cluster formation in the gas phase during electrospray ionization (ESI), however, the detailed mechanism is controversial so far. During ESI process, an ionic cluster is generated from solution phase to gas phase in three main steps : the creation of charged droplets, coulomb explosion and disintergration of the charged droplets, and the formation of gas phase analyte ions from the charged droplets. Aerosol science of today provides a clear demonstration of the first two steps. However, the final stage of the ESI process is still not completely understood, and there is currently debate regarding the mechanism by which ionic clusters are generated. It is generally agreed that small analyte ions adhere to the ion evaporation model (IEM), in which solvated ions are directly ejected from charged droplet surfaces, while large globular species are likely released to the gas phase via the charged residue model (CRM), in which free ions are formed by evaporating the final stage of the solvent shell. The distinction between IEM and CRM based on the size and shape of the analyte is ambiguous, though. Here, we have investigated formation of alkali halide (MX, M = Na, K, Rb and Cs, X = Cl, Br and I) cluster cations and anions using ESI-MS as it is considered to be ideal solute in that it is completely nonvolatile and it forms different size clusters, from small to large, as concentrations in the charged droplets increases during solvent evaporation process. Interestingly, we have observed the polarity- and droplet size-dependent halide selectivity on the formations of cluster ions.

Poster Presentation : **PHYS.P-187**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Multiphase nickel sulfides on metalloporphyrin for the selective benzoic acid production via electrochemical benzyl oxidation

Talshyn Begildayeva, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Nickel sulfides are amongst the best materials for electrochemical oxidation reactions, however, its performance in advanced oxidation of organic molecules can be shaded by the low selectivity toward value-added product such as benzoic acid. Herein in this work, a facile pulsed laser ablation in liquids (PLAL), solvothermal, and sonochemical methods were utilized to design tailored and selective electrocatalyst with multiphase nickel sulfides (NiS and Ni_3S_2) and nickel tetraphenylporphyrin (NiTPP) with 5, 10, and 15 wt.% mass loading. NiTPP acts as a conductive substrate for multiphase NiS nanospheres as well as assists in controlled oxidation of benzyl alcohol to benzoic acid. NiS-NiTPP10% composite affords lowest overpotential of ~435 mV in HER tests, ~320 mV in OER studies, exhibits the remarkable selectivity of 99.8% for benzoic acid with Faradaic efficiency of 98.3%. The composite shows the highest yield of benzoic acid (2.23 mM), when compared with other composites, bare NiS, or NiTPP. Overall, the joint effect of NiS and NiTPP in one composite eliminates the key drawbacks of the single materials and further enhances the strength.

Poster Presentation : **PHYS.P-188**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Efficient Molybdenum Derived Electrocatalysts Fabricated by Pulsed Laser Methods

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Mo-based electrocatalysts recently are considered as the promising replacement for the expensive platinum(Pt)-based materials in the hydrogen evolution reaction. However, the general synthesis methods such as solvothermal and pyrolysis require high temperatures and involve many hazardous chemicals during the process. Herein, Mo-based materials were successfully synthesized by eco-friendly and facile methods of pulsed laser ablation in liquids (PLAL) and pulsed laser irradiation (PLI). These methods ensure uniformity and the clean surface of the Mo-based electrocatalyst, which is beneficial for the enhanced HER performance. The morphology and composition of the obtained electrocatalysts were assessed by common SEM and SEM-EDS analyses. Structural features were studied by X-ray diffraction and Raman spectroscopy. Electrochemical tests prove Mo-based electrocatalysts to be suitable and durable material for the energy conversion applications.

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Laser-assisted Design of Pt-lignin Composites for Improved Hydrogen Fuel Production

Wonji Go, Talshyn Begildayeva[1], Seung Jun Lee[2], Myong Yong Choi[1,*]

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[2]*Department of Transportation Energy Convergence, Korea National University of Transportation, Korea*

The lignin is known as an environmentally friendly polymeric material that usually is extracted from biomass. Recently, lignin attracted attention due to its reducing and stabilizing properties in the synthesis of nanomaterials. These features are beneficial for the waste-free material fabrication, where lignin can replace harmful and highly reactive surfactants and reducing agents. Herein, pulsed laser irradiation technique was employed to obtain platinum (Pt) nanoparticles (NPs) functionalized with lignin, where latter helps to reduce Pt ions and further prevents Pt NPs aggregation. The physicochemical properties, structural, compositional and morphological features of the Pt-lignin composites were analyzed via ultraviolet(UV)-visible, XRD, SEM (SEM-EDS), and X-ray diffractometer. Performance of the Pt-lignin composites was assessed in a series of electrochemical hydrogen evolution reaction (HER), where it was proven to be an efficient electrocatalyst for the pure and zero-waste hydrogen fuel production.

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Poster Presentation : **PHYS.P-190**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Microstructural Uniformity Analyses of Annealed Poly(3-hexylthiophene) (P3HT) Films Using Raman Mapping

Jiyeong Park, Hyewon Kim, Jaeseong Heo, Myeongkee Park[1,*]

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

Poly(3-hexylthiophene) (P3HT) has excellent electrical conductivity, electroluminescence, and nonlinear optical properties. It has been used in a variety of applications, such as light-emitting diodes, organic field-effect transistors, and organic solar cells. Thermal annealing is an effective way to improve the electrical performance in P3HT films by enhancing crystallinity and structural homogeneity. However, the detailed microstructural information by the annealing process has not yet been understood. In this study, we have studied the temperature-dependent annealing effect and microstructural uniformity of P3HT films using Raman mapping. Among the Raman modes, we have focused on the in-plane ring skeleton mode at 1445 cm^{-1} which is assigned to the symmetric $C_\alpha=C_\beta$ stretching mode. This mode is sensitive to the delocalization of π-electron in the P3HT molecule. Thus, Figure 1(a) shows that the intensity at 1445 cm^{-1} increases while its width decreases (Figure 1a), as the annealing temperature increases. In addition, we have investigated that the uniformity of the P3HT film using Raman mapping with peak intensities and widths shown in Figure 1(b–e). As a result, we have found the highest structural uniformity in the film annealed at 100 ℃ (Figure 1c), which shows the highest Raman intensity and smallest width (data is not shown here).

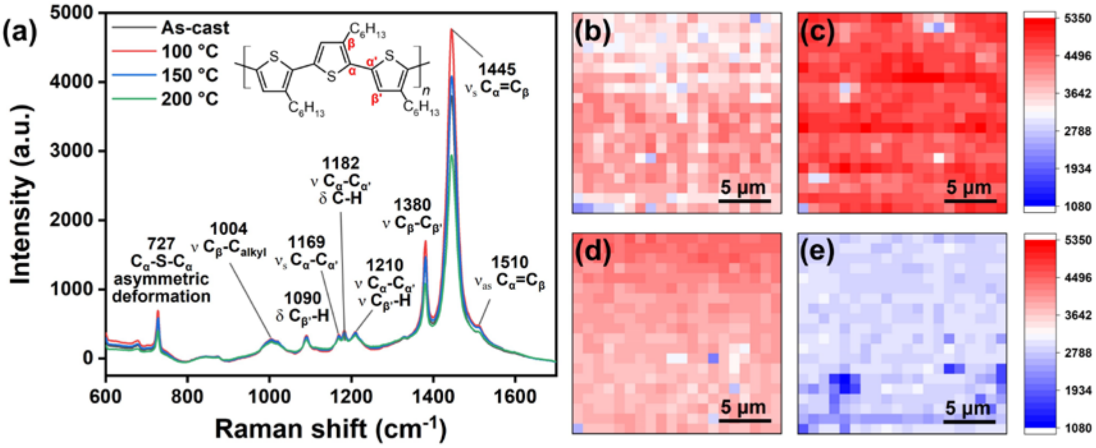

Figure 1. (a) Raman spectra of P3HT annealed at as-cast, 100, 150, and 200 °C, (b) Raman intensity maps of 1445 cm^{-1} peak at not annealed, (c) 100, (d) 150, and (e) 200 °C.

Poster Presentation : **PHYS.P-191**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Phase Transition of sub-10 nm Cesium Lead Bromide Perovskite Quantum Dots Studied by Temperature-dependent Raman and Photoluminescence Spectroscopies.

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

Lead halide perovskite quantum dots (QDs) have tunable band gaps, high extinction coefficients, narrow emission line widths, and long charge carrier diffusion lengths. On the other hand, inorganic cesium lead halide perovskite quantum dots, unlike other organic-inorganic perovskites, have better stability against heat and humidity, which is advantageous when used as solar cell devices or photocatalysts that directly or indirectly receive solar radiation. However, it is still highly unstable due to humidity and thermal energy, and it is difficult to synthesize it with a uniform size. In this study, we present uniformly synthesized sub-10 nm sized QDs and structural and optical properties using Temperature-dependent Raman and photoluminescence (PL) spectroscopies. $CsPbBr_3$ QDs can be synthesized in the temperature range of 100–180 °C using hot-injection method. As the injection temperature increases, the size of QDs increases. This leads to a red-shifted PL peak. In principles, as relatively less energy is emitted, the structural stability in QDs increases. We have found that the most stable and uniform QDs can be synthesized at 180 °C, compared to 140 ℃ and 160 ℃. The size of the QDs were measured to be 8.9 nm, and the maximum of PL peak was observed at 490 nm. We also measured temperature-dependent Raman and PL spectra with 10 °C intervals in the range of -150 °C to 150 °C. We have found that the phase transitions was observed 20 ℃ and 100 °C.

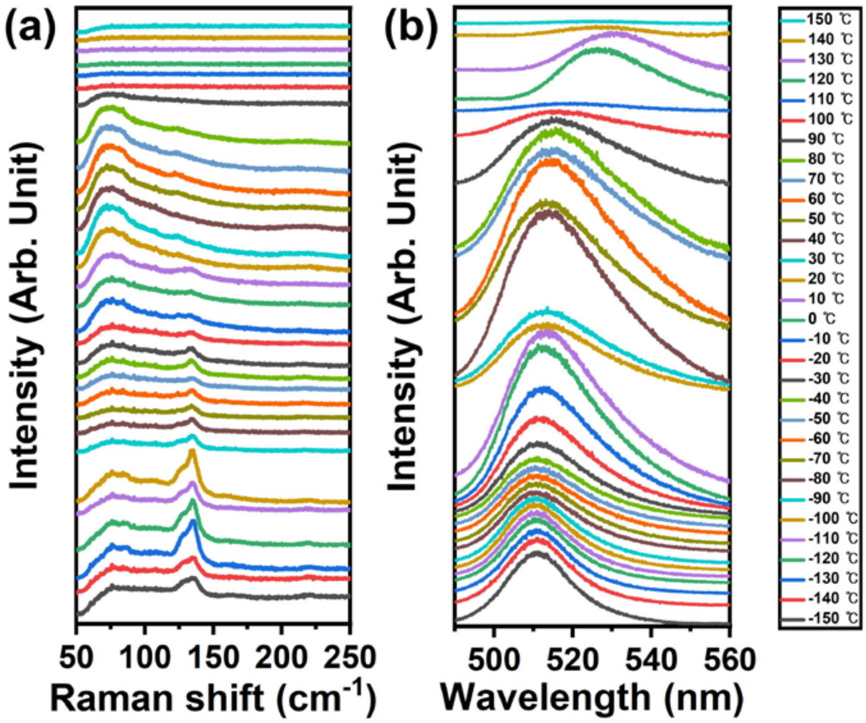

Figure 1. (a) Temperature-dependent Raman spectra and (b) PL spectra measured at 10 °C intervals from -150 °C to 150 °C.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Large-area Raman Analysis on Microstructural Homogeneity of Sulfuric Acid-Treated PEDOT:PSS Film

Hyewon Kim, Jiyeong Park, Jaeseong Heo, Myeongkee Park*

Department of Chemistry, Pukyong National University, Korea

PEDOT:PSS (Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate)) has been used as a transparent electrode because of its excellent conductivity and flexibility. To further improve the conductivity, the film can be treated with highly concentrated sulfuric acid, which increases the fraction of linear quinoid structures. Thus, it leads to greater electron delocalization and higher electron mobility in PEDOT. In this study, Raman spectroscopy was used to analyze the structural homogeneity of PEDOT:PSS film treated with sulfuric acid at various concentrations (Figure 1a). In addition, Raman mapping technique was used to determine the uniformity and crystallinity of the films. As the concentration of sulfuric acid increased, the intensities of the 1529 and 1562 cm^{-1} peaks decreased, indicating that the density of PSS decreased. We have observed the blue shift at around 1414 cm^{-1}, which was attributed to the C_α=C_β stretching vibrational mode. This blue shift indicates the transition from benzoid to quinoid structure. In addition, the widths of the peaks at 1414 cm^{-1} were 31.4 (0 % H_2SO_4), 33.6 (20 %), 31.1 (40 %), 32.5 (60 %), 30.9 (80 %), and 29.6 (100 %), determined by Gaussian fittings, suggesting that the PEDOT:PSS film treated with > 80 % sulfuric acid shows excellent crystallinities and uniformities.

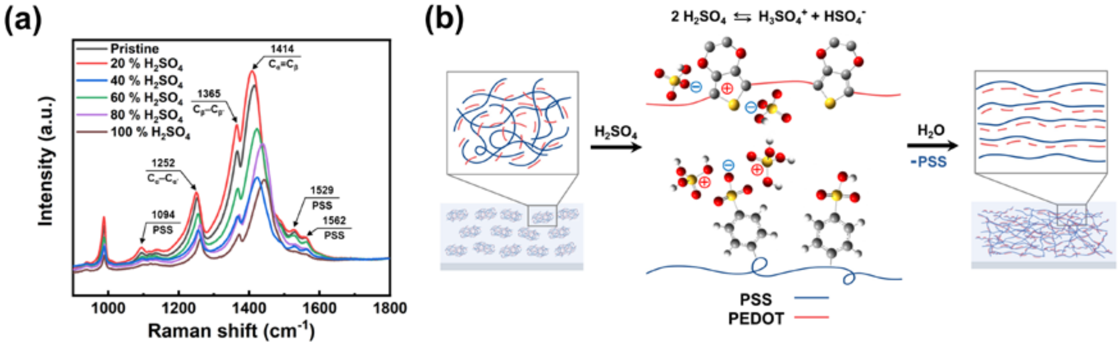

Figure 1. (a) Raman spectra treated with none, 20, 40, 60 ,80, and 100 % concentration H_2SO_4 and (b) diagram of the charge-separation structural change of PEDOT:PSS with addition of H_2SO_4.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Deep-UV Resonance Raman Spectroscopy of Exosome: Cancer Cell Line Screening

Ah-hyun Woo, Sila Jin[1], Yeonju Park[1], Jongmin Park[2], Young Mee Jung[*]

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[2]*department of Chemistry, Kangwon National University, Korea*

Recently, study on early cancer diagnosis and anticancer therapy monitoring using exosomes has become in the spotlight. Exosomes, which also exist in body fluids, reflect various cellular information. The cancer diagnosis method by exosomes is expected a promising sensitive diagnosis while reducing the pain of patients caused by biopsy. Raman spectroscopy is a powerful method for cancer diagnosis as it shows material-specific information in the finger print region, However, since most biological samples emit strong autofluorescence in regions above 260 nm, it is difficult to obtain biological sample spectra with visible light lasers. In this study, to overcome the autofluorescence of exosome, 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-194**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of carbon quantum dots using graphite, graphene oxide, and lignin sources via pulsed laser ablation in ethanol

Haeun Kim, Yu Jeong Jeong, Seung Jun Lee[1], Myong Yong Choi*

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[1]*Department of Transportation Energy Convergence, Korea National University of Transportation, Korea*

In this study, carbon quantum dots (CQDs) were successfully produced using graphite powder, graphene oxide, and lignin sources via pulse laser ablation (PLA) in ethanol as solvent. Ascorbic acid used as a reducing agent. The PLA reaction was performed by using a Nd:YAG pulsed laser (Surelite II-10) with a wavelength of 1064 nm and a laser power of 200 mJ for 20 min. The formation and fluorescence properties of the synthesized CQDs were analyzed using various analytical techniques such as UV-Vis, PL, and TEM. CQDs are chemically stable as carbon nanoparticles exhibiting quantum effects and have no biotoxicity, so they are emerging as next-generation luminescent substances to replace organic luminescent and semiconductor quantum dots. The synthesized carbon quantum dots are several nm in size, have different colors depending on the size of the particles, change the fluorescence wavelength depending on the size of the particles, and have typical quantum dot characteristics that emit fluorescence of different wavelengths. Also, CQDs are bio-friendly carbon compounds, so they can be applied to sensors that can be injected into the human body.

Poster Presentation : **PHYS.P-195**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Interface engineering of Mo-doped NiO@Ni with strong heterostructure boosting oxygen evolution reaction and urea oxidation

Maheskumar Velusamy, Myong Yong Choi[1,*]

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The design and implementation of affordable high-performance electrocatalysts for the oxygen evolution reaction (OER) and urea electrooxidation reaction (UOR) are critical for clean and environmentally friendly energy conversion. In this study, we report the electrocatalytic performance of a novel heterostructure interface engineering of Mo-doped NiO@Ni (Mo-NiO@Ni) for the high electrocatalytic activity of OER and UOR. Structural and morphological analyses confirmed the formation of a Mo-NiO@Ni heterostructure interface. The optimized Mo-NiO@Ni demonstrated electrocatalytic performance with low overpotentials of 320 mV at 10 mA cm−2 for OER and 1.382 V vs. RHE at 50 mA cm^{-2} for UOR with better stability after testing for 12 h. Mo dopants can effectively increase the conductivity and electrochemical active surface area of NiO@Ni and simultaneously enhances the intrinsic OER and UOR activity. Interestingly, Mo-NiO@Ni was successfully employed as anode for urea-assisted water electrolysis and verifying the lower energy consumption during electrolysis. This work provides a viable strategy to solve the energy challenge.

Poster Presentation : **PHYS.P-196**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

In-situ growth of noble-metal doped $Ni(OH)_2$ on Ni foam via pulsed laser irradiation for an effective electrochemical total water splitting

Jangyun Kim, Yu Jeong Jeong, Seung Jun Lee[1], Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Department of Transportation Energy Convergence, Korea National University of Transportation, Korea*

Hydrogen obtained from water electrolysis is attracting attention as a sustainable and carbon-neutral energy source. The electrolysis reaction of water includes a hydrogen evolution reaction (HER) and an oxygen evolution reaction (OER), and OER requires 1.23 V compared to RHE, which is regarded as an obstacle in highly efficient water electrolysis reaction. Therefore, research on lowering the overpotential of the OER is being conducted for a highly efficient water electrolysis reaction. Ni foam has abundant reserves and a large surface area with a 3D porous structure, so it has high conductivity and has the advantage of being directly used as an electrode. In this study, $Ni(OH)_2$ growth on Ni foam was successfully achieved via pulsed laser irradiation (PLI) of Ni foam as target in a 1.0 M KOH solution. However, the HER and OER activities of $Ni(OH)_2$ / Ni foam were rather poor in alkaline media. Therefore, the various noble-metal was introduced into $Ni(OH)_2$ / Ni foam (M-$Ni(OH)_2$ / Ni foam, where M=Ir, Ru, and Pd) by the PLI of the corresponding noble metal salts. The prepared catalysts were intended to be used for HER and OER reactions. The Ru-$Ni(OH)_2$ / Ni foam sample achieved the lowest potential of 90 mV (HER) and the Ir-$Ni(OH)_2$ / Ni Foam sample achieved the lowest potential of 335 mV (OER). As a result, it was confirmed that the Ir-$Ni(OH)_2$ / Ni foam catalyst would act as an effective bifunctional catalyst for the water electrolysis reaction.

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Poster Presentation : **PHYS.P-197**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photocatalytic NO oxidation by Fe-TiO_2 combined with surface hardening agents cement blocks: impacts of Fe-TiO_2 contents in coating solutions

Shufang Zhao, Young Dok Kim[1,*]

chemistry, Sungkyunkwan University, China
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Photocatalytic activity of commercial TiO_2 particles (R996) towards NO oxidation under visible light irradiation at 50RH% can be enhanced by a temperature chemical vapor deposition of Fe-oxide (0.4 wt%) and post annealing (375 ^{o}C, 2 hrs). Fe–TiO_2@SHA/cement block samples were prepared by dispersing the modified TiO_2 particles (Fe–TiO_2) on cement blocks using a surface hardening agent (SHA) as a binder. The Fe–TiO_2@SHA/cement blocks exhibited higher photocatalytic activity in promoting the conversion of NO into NO_3–$^-$ than the particulate counterparts. The Fe–TiO_2@SHA/cement blocks exhibited dissimilar patterns in terms of the changes in NO removal as a function of the reaction time in the early stage of the reaction (0–150 min) depending on the Fe–TiO_2 contents. The removal of NO increased gradually as the reaction time increased with lower Fe–TiO_2 contents, whereas a gradual decrease in NO removal as a function of the reaction time was observed with higher Fe–TiO_2 contents. The dependence of the response on the Fe–TiO_2 contents was attributed to the dissimilar Fe–TiO_2 structures formed on the cement blocks due to variations in the viscosity of the Fe–TiO_2 coating solutions with different Fe–TiO_2 contents.

Poster Presentation : **PHYS.P-198**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chiral-Induced Surface-Enhanced Raman Optical Activity on Nanoparticle-on-Mirror Substrate

Sung Gun Lee, Dae Hong Jeong[*]

Department of Chemical 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-199**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Peptoid-scaffolded Diphenlyanthracene Dimers for Intramolecular Triplet-Triplet Annihilation Upconversion: Photochemical Properties and Influence of Molecular Geometry

Dongcheol Park, Hohjai Lee[1,*]

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

- Withdrawal -

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Removal of benzene and ammonia gases with activated carbon under visible light irradiation.

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

Removal efficiencies of benzene and ammonia were examined using as-received commercial activated carbon (AC) at 0%, 30%, and 60% relative humidity (RH) with and without visible light irradiation. We demonstrated that light improved the removal efficiency of benzene even when nitrogen was present, and the improvement impact was more when H_2O and O_2 were present. We also showed that, under ideal humidity levels, visible light irradiation can increase the ammonia removal effectiveness. We further proposed NH_3 movement that is more effectively aided by light and water through the nanoporous channels of AC. The oxidizing agents, such as OH radicals produced by light irradiation and other reagents, changed the surface structure of AC. These modifications were studied using Fourier-transform infrared (FT-IR) studies.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Aggregation of Fe(II) and Fe(III) Protoporphyrin IX in the Gas Phase

Yunseop Choi, Jongcheol Seo*

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

Porphyrin is a heterocyclic molecule that has aromaticity that can make aggregation structure by π-π stacking interaction. Among the various porphyrin, protoporphyrin IX (PPIX) has unique aggregation properties in the gas-phase through hydrogen bonding of propionic acid groups and π-π interaction. Meanwhile, metalloporphyrin is a molecule that metal atom binds to the porphyrin center. One of the famous metalloporphyrins is Fe(II)PPIX in hemoglobin, which plays a significant role in oxygen transport in vivo. FePPIX can also make aggregation in the gas-phase by π-π stacking. The aggregation properties of these porphyrins are essential because they receive great attention in supramolecular chemistry and porphyrin nanostructures. In this study, we investigated the aggregation behavior of PPIX and hemin, including Fe(III)PPIX, in the gas-phase using ion mobility spectrometry-mass spectrometry (IMS-MS). The oligomers containing both molecules were well observed in MS. Investigating the aggregation behavior of Fe(III)PPIX and PPIX suggests the influence of metal center on their aggregation properties. In addition, the difference between the aggregation made by PPIX with Fe(III)PPIX or Fe(II)PPIX, reduced from Fe(III)PPIX, was compared to explore the effect of the oxidation state of metal atoms in aggregation. Finally, additional DFT calculation was performed to identify the experimental results and specific structural analysis.

Poster Presentation : **PHYS.P-202**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Machine Intelligence Approach in Physicochemical Feature Optimization

You Kyoung Chung, Joonsuk Huh*

Department of Chemistry, Sungkyunkwan University, Korea

The prediction of efficient and accurate aqueous solubility of the drug-sized compound is highly desirable in the chemical and pharmaceutical industries. However, solubility prediction remains a critical challenge in drug delivery and development. With the advent of Machine learning (ML)-based tools in technology, artificial intelligence (AI) approaches have become increasingly popular for the design of drug-like molecules and the analysis of quantitative structure-property relationship (QSPR) for drug discovery. Here, we present a deep learning Quantitative Structure-Property Relationship (QSPR) model that is fundamentally integrated with deep neural networks (DNNs) and auto feature optimizer (AFO) to construct the parameter search space dynamically, reduce the complexity of deep learning method with the cumbersome hyperparameter search, and build the efficient implementation of both searching and pruning strategies. Using this method, we predict the intrinsic solubility of 3475 organic compounds from 4 different data sets. The most suitable set of molecular features is selected in auto-optimization, and an accurate final model is developed with the hyperparameter optimization process.Furthermore, our new predictive model demonstrated state-of-art performance, with the highest accuracy of 99.1 for ESOL data, compared with the standard models, such as ridge regression (RR), support-vector machines (SVMs), and multi-layer perceptrons (MLPs), as well as deep neural networks (DNNs). We also show the performance of the three combined fingerprints (Morgan, MACCS key, and Avalon) in the physicochemical feature optimization. Based on an analysis of feature importance, we identified that the essential properties of molecules on solubility prediction are molecular weight (molecular weight), TPSA (total polar surface area), Log P (partition coefficient ratio of substances in the water to octanol solvent), and Mol_MR (polarizability), and electron density (Estates). These results are well consistent with other studies. Thus, this study potentially implies that our ML method is outstanding for increasing the accuracy of predictive modeling of physical properties, applying automated modeling or feature selection for new chemistry data, and making the principles of the predicted model explainable to advance the discovery of new materials.


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Poster Presentation : **PHYS.P-203**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chiral-Selective Cluster Ion Formation of Glucoses and Serines in the Gas Phase

Doui Kim, **Jongcheol Seo**[1,*]

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

Studying stable chiral-selective biomolecular aggregates is valuable because it can help us understand how nature achieves homochiral selectivity and chiral transfer. Amino acids and sugars are particularly interesting since they often exhibit unique homochiral selectivity. For example, the homochiral serine octamer ion has a highly-oriented symmetric molecular arrangement, which has been successfully observed and characterized by mass spectrometry in the gas phase. In the present work, we have extended our research on stable chiral-selective biomolecular aggregates to a heteromolecular system containing serine/sugar complexes. The study observes a unique cluster anion composed of three serine, two glucose, and a chloride ([Ser3Glc2Cl]-) using electrospray ionization-mass spectrometry (ESI-MS). This cluster anion is only formed homochiral, with either L-serine/L-glucose or D-serine/D-glucose combinations. The study shows that substituting the serine with other amino acids or the glucose with other hexoses did not yield the same cluster ion. The unique observation of this cluster anion suggests the need for further structural determination, indicating the structural distinctiveness of these serine/glucose/chloride complexes.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Thickness dependent diffusional heterogeneity of water molecule confined between lipid bilayers

Minho Lee, Ji-Hyun Kim, Minhaeng Cho[1], Jaeyoung Sung[*]

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

The transport dynamics of water confined between lipid bilayer membranes, also known as hydration water, differ significantly from those of bulk water due to the interaction between water molecules and lipid head groups. While the mean square of lateral displacement (MSD) of hydration water has been widely studied, the non-Gaussian character of its transport dynamics, reflecting the diffusional heterogeneity of water motion, has not yet been quantitatively analyzed. In this work, we use molecular dynamics simulations to study the non-Gaussian transport dynamics of water molecules confined between 1,2-dimyristoyl-sn-glycero-3-phosphorylcholine (DMPC) bilayer membranes. To control the thickness of confined water, we adjust number of confined water molecules.By analyzing the MSD and non-Gaussian parameter (NGP) for lateral water displacement, we extract and quantify the environment-coupling dynamic heterogeneity of water molecules (DKC). This value can be described as the time correlation function of diffusion coefficient fluctuation at long times. As the thickness of confined water increases, the relative variance of diffusion coefficient decreases, but this decrease is accompanied by a slower decay.Through our research, we found bulk-like water layer with similar properties to bulk water. As the thickness of confined water increases, portion of bulk-like water layer increases, resulting in a decrease in the relative variance of the diffusion coefficient. This is because the dynamic heterogeneous of bulk-like water layer is ignorable. At the same time, bulk-like water layer hinders the transfer of water molecules between interfacial water layers on either side of this layer. That is why the relaxation time of DKC increases as the thickness of confined water increases.

Poster Presentation : **PHYS.P-205**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Protomers of imipramine captured by the host-guest chemistry with cucurbit[7]uril

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

Various small molecules with multiple protonation sites commonly carry out important functions in our body. Protonation site of those molecules can change their physiological properties. However, protonation isomers (protomers) are often hard to discriminate because of their negligible structural difference. In this work, we distinguished two protomers of imipramine by introducing cucurbit[7]uril (CB[7]) using electrospray ionization ion mobility spectrometry combined with mass spectrometry. Imipramine is a widely used for anti-depression treatment, which has two amine group on cycloheptadiene ring and side chain, respectively. Protomers of imipramine form host-guest complexes with CB[7], and the difference of collision cross section (CCS) between two complexes becomes significant during electrospray ionization process. A few stable structures of complexes were expected by density functional theory, and their theoretical CCS values accord with experimental values. Moreover, the host-guest interaction enables to capture less favorable protomer. This work suggests a new strategy of separating small molecules with insignificant structural differences by host-guest chemistry.

Poster Presentation : **PHYS.P-206**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Structure of water molecules in carbon nanocones: Molecular Dynamics Simulations

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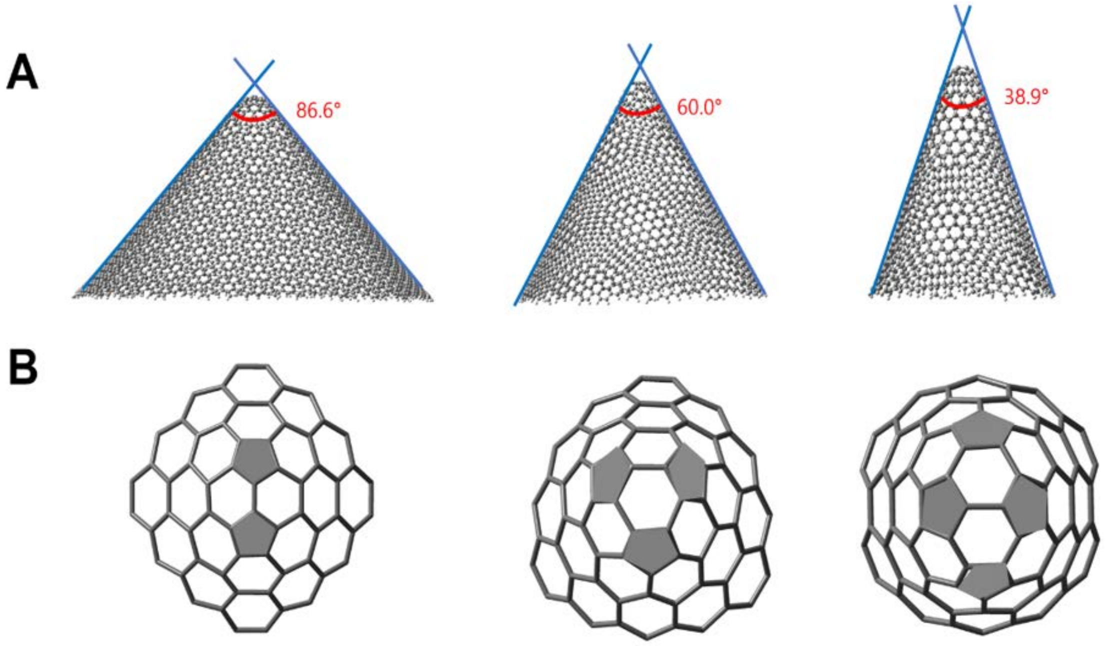
Department of Chemistry, Sejong University, Korea

Nano-confined water possesses unique physical and chemical properties, which make it suitable for various industrial applications such as fluid reservoirs, gas separation, water desalination, DNA detection, and drug delivery. As a result, comprehending the structural and dynamic properties of fluids, particularly water, in nano-confinement materials is of fundamental importance. Numerous studies have shown that different phases of water coexist in carbon nanotubes (CNTs). The order of phase change is vapor, ice-like, and liquid as the position changes from the carbon walls. Typically, the phase boundary is divided by the water density in CNTs.The carbon nanocone (CNC) exhibits gradual changes in water confinement in one system, ranging from extreme confinement near the tip of the CNC to a bulk-like environment as it moves away from the tip. In this study, we demonstrated the coexistence of different water phases in the CNC using molecular dynamic simulations. We also compared the variations in water structure, not only within the CNC, but also between CNCs of different shapes, i.e. the peak angle of the CNC.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Poster Presentation : **PHYS.P-207**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Gas-Phase Cyclodextrin Aggregation with Alkali Halide Cluster Ions

Yunyoung Ahn, Jiyeon Lee[1], Jongcheol Seo[1,*]

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

Cyclodextrins (CD) have both the hydrophilic and hydrophobic moieties and they gather themselves together to form a cluster. These self-assembled clusters have been investigated in advanced applications, including drug delivery, selective binding, and controlled adsorption. However, the studies on the CD aggregation behavior seem to be sparse and little is known about the structure of self-assembled CD with small molecule guests. In the present work, the aggregation behavior of cyclodextrins with alkali metal chloride clusters has been investigated by ion mobility spectrometry–mass spectrometry (IMS-MS). Observed CD multimers such as trimer and tetramer with alkali metal chloride clusters showed multiple structures depending on the position of salt clusters. Interestingly, at some point CCS become smaller even when salt cluster is added, which means certain multimers are making compact and stable structure. Especially, tetramer formed stable symmetrical structure compared to odd number of complexes such as trimer and pentamer. The collision-induced dissociation (CID) results further demonstrated that this tetramer forms symmetric structure around halide ions. Further modeling study is ongoing to discover how this stable complex is constructed.

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Poster Presentation : **PHYS.P-208**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Why effective core potential (ECP) basis sets fail in optimizing excited state structures of complex containing Hg2+ ion

Dae-Hwan Ahn, Jong-Won Song*

Chemistry Education, Daegu University, Korea

Recently, we performed the time-dependent (TD) density functional theory (DFT) calculations on the tetraphenylehtene – bis(thiophen-2-ylmethyl)amine (TPE-BTA) which shows a turn-on bright green fluorescence along with high sensitivity toward Hg2+ to discover the structures of TPE-BTA complex with Hg2+. However, we found that only x2c-TZVPPall, all electron (AE) basis set, for the Hg2+ ion successfully reproduces the absorption and vibrationally resolved fluorescence spectra close to the experimental spectra, but all the tested effective core potential (ECP) basis sets, such as Lanl2DZ, CRENBL, def2-TZVP, and aug-cc-pVTZ-PP, failed to optimize the excited state geometries related to the fluorescence spectra calculations [1]. In addition, ECP basis sets provided too small fluorescence energies during optimization process of the first excited state. Hence, in this presentation, we studied why ECP basis set totally failed to calculate the optimized structures containing Hg ion. We found that at least the system containing Hg2+ ion should be calculated using all electron basis set to escape from geometrical erroneous behavior coming from ECP basis sets. The reason for this is that ECP basis sets provide the rapidly decreased HOMO-LUMO gaps with the distance between ligand and Hg2+ increased whereas x2c-TZVPPall calculates gradually decreasing HOMO-LUMO gaps. Furthermore, ECP basis sets calculate too weak binding energies between the ligand and Hg2+.[1]. M. Selvaraj, K. Rajalakshmi, D.-H. Ahn, S.-J. Yoon, Y.-S. Nam, Y. Lee, Y. Xu, J.- W. Song, K.-B. Lee, Anal. Chim. Acta 1148 (2021), 238178.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Bromine and Hydroperoxyl Radical Formations via BrO_2H photodissociation

Svetlana Shostak, Cheol Ho Choi*

Department of Chemistry, Kyungpook National University, Korea

Using quantum mechanical methods, the formation of XO_2H species (where X is F, Cl, or Br), which are precursors to halogen and hydroperoxyl radicals ($O_2H\cdot$), has been studied. In the case of BrO_2H, the strong spin-orbit coupling (SOC) makes it easy for the initial triplet species to cross over to a more stable singlet species. As a result, the formation of singlet BrO_2H is highly likely, which can then undergo exothermic photo-dissociation to produce $Br\cdot$ and $O_2H\cdot$ (the bright channel). Conversely, the less energetically favorable triplet species are loosely bound and can be easily subjected to thermal dissociation, resulting in the formation of $Br\cdot$ and $O_2H\cdot$ (the dark channel). In essence, the bright and dark channels represent two alternative pathways for the formation of $Br\cdot$ and $O_2H\cdot$ radicals.

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Computer Simulation of Stretchability in PEDOT:PSS Film with Ionic Liquid

Changwon Choi

Daegu Gyeongbuk Institute of Science & Technology, Korea

A conducting polymer, poly(3,4-ethylenedioxythiophene):poly(stryrenesulfonate) (PEDOT:PSS), is attracting great attention for various applications such as organic light-emitting diodes, solar cells, thermoelectric generators, self-powered sensors, and artificial skin, owing to its low cost, solution processability, and flexibility. Pristine PEDOT:PSS films have poor electrical conductivity, but it can be improved by adding specific ionic liquids (ILs) through a morphology control. Such well-ordered PEDOT nanostructures help charge transfer, but suffer from poor elasticity. Therefore we now focus on how these ILs affect the mechanical properties of PEDOT:PSS at the molecular level through molecular dynamics simulations. We build amorphous film models of PEDOT:PSS with and without ILs, simulate their strain by stretching these films at a constant rate in the axial direction, and define the stress as the pressure tensor during deformation. The simulated strain-stress relationship shows that the IL improves the elasticity of the film. The principles of improving the mechanical properties of ILs are identified and IL design principles for elasticity control are proposed.

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Poster Presentation : **PHYS.P-211**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Valence molecular orbitals and the cationic structures of difluoropyridine derivatives by high-resolution VUV-MATI mass spectroscopy

Hyojung Kim, Sung Man Park, Chan Ho Kwon*

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

Halopyridine has received considerable attention because substitution of hydrogen with halogen atom in pyridine affects the energy ordering of the valence orbitals. In addition, the effect of the position and the number of the halogen atom on pyridine ring, which ultimately affects the corresponded cationic states, has been investigated by various ion spectroscopies. In the previous investigations on 2-fluoro- and 3-fluoro-pyridines, it was found that the stability of the nonbonding orbital commonly increases due to the considerable interactions between the lone-pair *p* orbitals on the nitrogen and those of adjacent fluorine atom, resulting in the generation of the reversed order with the σ_N and π orbitals of pyridine. Further, the energy gap between the two lowest cationic states for 2-fluoropyridine increased because of the efficient interaction among the orbitals from the nitrogen and fluorine atoms in *ortho* position. Thus, we explored the valence orbitals and the corresponded cationic structures of difluoropyridine derivatives utilizing high-resolution vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) mass spectroscopy and the Franck-Condon analysis.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Observation of Ultrafast Charge Transfer Dynamics in Hetero-Bilayer Transition Metal Dichalcogenides by Pump-Probe SHG Spectroscopy

Juseung Oh, **Sunmin Ryu**[1,*]

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

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Detection of benzenediol compounds with SERS using Metal-Chelation Nanoshell(MCNS)

Mingyeong Kim, Yun Sik Choi, Dae Hong Jeong*

Department of Chemical Education, Seoul National University, Korea

Surface-enhanced Raman Spectroscopy (SERS) is an outstanding spectroscopic analytical technology that shows high sensitivity and specificity. However, the detection of molecules with SERS mostly depends on the interaction between metal and analyte molecules. Thus, detecting molecules such as non-thiol compounds which lack attractive interaction with metals in an aqueous solution is challenging so far. In this research, we utilized Metal-Chelation to detect benzenediol compounds, including 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 ions by coordinate bonds between hydroxyl groups and metal ions. To effectively detect DA and catechol, we optimized the reaction procedure by changing metals (Cu, Zn) and capping agents (2-mercaptoethanol and PVA). Finally, we successfully detected dopamine (DA) and catechol with MCNSs in various aqueous solutions, including DW and MgSO4 buffer.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Top-Down Approach for Two-Dimensional Tetracene Molecular Crystals Studied with Polarized Reflectance and Photoluminescence

Jonghyun Son, Sunmin Ryu[1,*]

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

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

In this work, we report on a top-down approach to form two-dimensional (2D) organic molecular crystals and a thorough spectro-imaging analysis. The conventional methods [1, 2] involved the use of physical vapor deposition on inorganic 2D crystal templates, however mechanical exfoliation [3], which is used to produce many inorganic layered crystals, might also be utilized to create high-quality few-layer molecular crystals on arbitrary substrates. We performed topography absorption and photoluminescence (PL) measurements on 2D tetracene (Tc) crystals to contrast the two methods. Wide-field PL imaging was also exploited to map their crystallographic orientations. Polarimetric analysis based on two orthogonal polarization components revealed long-range order that spanned more than several microns for both crystals. Mechanical exfoliation, which can prepare single-crystalline bulk to 2D molecular crystals, may be a powerful method to study optical properties depending on thickness.

Poster Presentation : **PHYS.P-215**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Charged-GFP aggregation (or liquid-liquid phase separation) in a polyamine-deficient E-coli

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Department of chemistry, Pusan National University, Korea

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

Most proteins that exhibit aggregation or phase separation in cells are charged. In our previous report, we showed that small charged molecules are necessary to form charged-protein aggregates. We also found that multivalently charged small molecules play a critical role in making protein aggregates when the proteins are charged, by acting as a bridge between multiple proteins. While we confirmed this result in E. coli, we were unable to rule out the role of endogenous polyamine molecules in the process. To investigate this further, we used a polyamine synthetase knock-downed E. coli strain (HT873) to examine the role of polyamines in the aggregation of negatively (-27) and positively (+28) charged GFP. Our results showed that in the HT873 strain, the phase separation of positively charged GFP was 40% more frequent than in the normal E. coli strain because endogenous negatively charged small molecules (NTP) were not disrupted by polyamine molecules. In contrast, the behavior of negatively charged GFP was similar to our previous study, in which phase separation occurred after polyamine treatment. These findings suggest that charged small biomolecules play a critical role in the phase separation of charged proteins in cells.

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Poster Presentation : **PHYS.P-216**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Spectroscopic study of Methylbenzyl radicals in a corona excited supersonic expansion

Changsoon Huh

Department of Applied Chemistry, Dong-Eui University, Korea

We report the spectroscopic and ab initio and spectroscopic evidence of the 1, 3, 5- trimethylbenzyl and 3, 5-dimethylbenzyl radical in corona excited supersonic expansion(CESE). The electronically hot but jet-cooled 1, 3, 5- trimethylbenzyl and 3, 5-dimethylbenzyl radical has been produced from precursor 1, 2, 3-trimethylbenzene seeded in large amount inert carrier gas helium by using the technique of CESE with a pinhole-type glass nozzle. AB initio calculation were carried out with the GAUSSIAN-09 package and vibronic emission spectrum of the 3,5-dimethylbenzyl radicals were recorded with a long path monochromator in the D1 → D0 electronic transition in the visible region. Ab initio calculation of the ground-state benzyl radical have been carried out with density functional method and the complete basis set model. The observed spectrum is consistent with the result of vibrational frequencies of the ab initio calculation and the benzyl radical ground state reaction mechanism through the hydrogen migration is presented. Furthermore, the ab initio calculation explains the benzyl radical generation mechanism in the excited state through the anti-bonding energy surface.

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Poster Presentation : **PHYS.P-217**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Design strategies for a compact 3D imaging spectrometer in spectroscopic nanoscopy

Ki-Hee Song

Quantum Optics Research Division, Korea Atomic Energy Research Institute, Korea

Spectroscopic nanoscopy has been recognized as an essential tool in functional super-resolution imaging as it offers spatial and spectral information of single molecules at nanoscale resolution. A recently developed dual-wedge prism (DWP) three-dimensional (3D) imaging spectrometer, a monolithic optical component, has broadened the accessibilities of spectroscopic nanoscopy with improved imaging resolution and system reliability. In this work, we present the design strategy of the DWP imaging spectrometer given the primary design parameters, such as the refractive index, spectral dispersion, axial separation, and the dimensional constraints. We show achievable spectral dispersion and localization performance for different design cases. This will give quick guidance for users to easily implement 3D spectroscopic single molecule imaging.AcknowledgementsThis work was supported by the National Research Foundation of Korea grant funded by the Korea government (MSIT). (No. NRF-2022R1C1C1002850)

Poster Presentation : **PHYS.P-218**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Conformer-Specific Spectroscopy of Cryogenic Protein Ions in the Gas Phase

Iltae Yoo, Jinho Jeong[1], Nam Joon Kim[2,*]

chemistry, Chungbuk Natioanl University, Korea
[1]*Chemistry, Chungbuk Natioanl University, Korea*
[2]*Department of Chemistry, Chungbuk Natioanl University, Korea*

The structure of protein molecules is one of the most popular fields in chemistry. However, the structures and distinguishing of conformers of gaseous cryogenic protein ions are still a mystery. Here, we have obtained the charge state and conformer-specific UV spectra of cryogenic apo-myoglobin and ubiquitin ions produced by electrospray ionization. The nitrogen tagging and dissociation technique was used to record the UV spectra of protein ions. Furthermore, a pump-probe method was used to record the conformer-specific UV spectra. Our study expands the range of the molecules in the cryogenic ion gas phase and opens the way to the cryogenic spectroscopy of huge proteins.

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mesoporous TiO2 particles synthesized via template free sol-gel method: efficient toluene removal with high resistance towards the benzoic acid accumulation

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Department of Chemistry and Energy Engineering, Sangmyung University, Korea

Template-free sol-gel methods may be a simple and cost-effective way to synthesize mesoporous particles since voids can be formed during the aggregation of TiO2 nano seeds. However, the difficulties in the control of size and shape of resultant particles and size distributions of mesopores made them less attractive as potential methods for the synthesis of mesoporous particles. In this work, the mesoporous TiO2 crystalline particles (diameter: 200-400 nm, pore size: 4-8 nm) having a high surface area (196.2 m2/g) were successfully synthesized via a simple sol-gel method without using any soft- and hard-template agents. The prepared mesoporous TiO2 particles can effectively remove gaseous toluene under UV light irradiation and have high resistance towards surface poisoning due to recalcitrant reaction intermediates, such as benzoic acid. The TiO2 particles were analyzed by means of various techniques, such as SEM, XRD, UV-DRS, PL, XPS, ex-situ FT-IR, HPLC, and operand DRIFT. And the analysis results allowed us to understand the origin of the high photocatalytic activity of the prepared TiO2 particles (high surface area, high electron-hole separation efficiency, coexistence of amorphous phase with anatase phase).

Poster Presentation : **PHYS.P-220**

Physical Chemistry

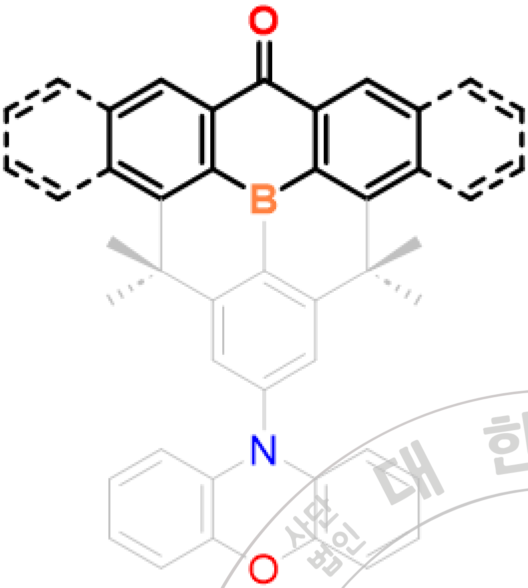
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Theoretical Investigation on Local Triplet Excited States and Unusual Emission Tuning of TADF molecules Based on π-Expanded Boron-Carbonly Hybrid Acceptors

Taehwan Lee, Chaerin Kim, Min Hyung Lee[1,*], Jaehoon Jung[1,*]

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

The photophysical properties of three donor-acceptor-type thermally activated delayed fluorescence (TADF) emitters (PXZBAO (1), PXZBTO (2), and PXZBPO (3)) are herein investigated using time-dependent density functional theory (TDDFT) calculations, which were comprising a phenoxazine (PXZ) donor and differently π-expanded boron-carbonyl (BCO) hybrid acceptor units.[1] Photoluminescence experiments revealed that the emitters exhibit red (1) to orange (3) emissions with an increase in the π-expansion in the BCO acceptors. This unusual emission color shift can be explained by the LUMO energy level of TADF emitter, which is attributed to the strength of local aromaticity for the π-expanded unit of BCO acceptors, for which the squared effective ring electron density (ERED^2) was evaluated as a descriptor for the local aromaticity of a ring over all Kekulé structures based on WFRT analysis. Also, To provide the photophysical insights of their TADF processes, we evaluated the spin orbit coupling matrix elements (SOCME) between the S_1 and T_n(n = 1 and 2) excited states. The SOCME between the S_1 and T_1 states is much larger than that between the corresponding S_1 and T_1 states for all compounds, as expected by El-Sayed rule. Consequently, all the emitters exhibit strong spin orbit coupling between their T_2 and excited singlet (S_1) states, leading to a fast RISC with rate constants of ~$10^6 s^{-1}$. We believe that our study will be useful for the design of D-A-type TADF emitters with fast RISC and controlled photophysical properties.[1] I. I. Nur, J.-H. Jang, T. Lee, Y. H. Lee, C. Kim, J. Jung, J.-H. Lee, and M. H. Lee, ACS Appl. Mater. Interfaces, in revision (2023)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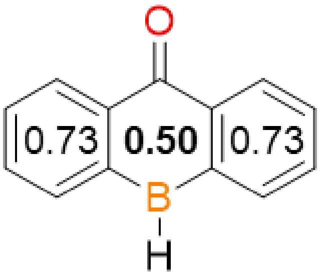
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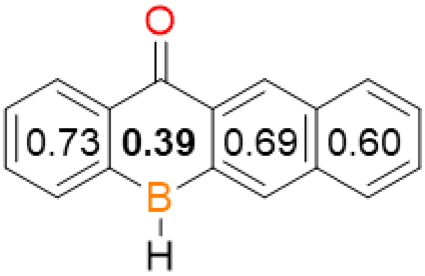
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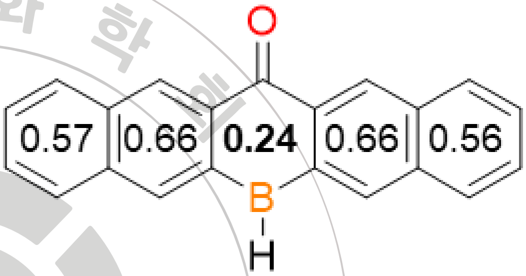
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Poster Presentation : **PHYS.P-221**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Universal critical behaviors in electrical conductivity of percolating clusters of hard spheres in continuum space

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In this study, we investigate the universal critical electrical transports of the percolating clusters in a three-dimensional continuum space. We generate the electrical clusters in continuum space by randomly distributing hard spheres without overlap in three-dimensional continuum space and considering two hard spheres to be electrically connected if their distance is less than a cutoff length scale r_{cut}. Using the finite-size scaling method, we precisely determine the volume fraction at percolation threshold φ_c, at which the percolating cluster of the electrically connected hard spheres emerges. We then calculated the electric conductivity of the percolating clusters using Kirchhoff's law for $\varphi \leq \varphi_c$ with varying the system size L from ~10 to ~250 containing ~10^2 to ~10^6 hard spheres. We find that when the correlation length ξ is greater than the system size L, the electrical conductivity Σ vanishes with increasing L, i.e., $\Sigma \sim L^{-\mu_1/\nu}$, where ν is a scaling exponent for ξ ($\xi \sim (\varphi-\varphi_c)^{-\nu}$). On the other hand, when ξ 〈L, Σ depends on φ and φ_c following a scaling relation, $\Sigma \sim (\varphi-\varphi_c)^{\mu_2}$. We discovered that the values of μ_1 and μ_2 were not affected by changes in r_{cut}, indicating universal scaling behaviors of the electrical conductivity. Interestingly, however, we find that μ_1 and μ_2 have different values beyond error ranges with μ_1=1.912 and μ_2=1.635, respectively, although they should be identical according to the percolation theory. Our findings imply that the transport exponent in the continuum space might be influenced by the measurement techniques.

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Poster Presentation : **PHYS.P-222**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A universal perovskite nanocrystal ink for dual-mode optoelectronic devices

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[1]*School of Chemical Engineering, Sungkyunkwan University, Korea*

Semiconducting lead halide perovskite nanocrystals (PNCs) are regarded as promising candidates for next-generation optoelectronic devices due to their solution processability and outstanding optoelectronic properties. While the field of light-emitting diodes (LEDs) and photovoltaics (PVs), two prime examples of optoelectronic devices, has recently seen a multitude of efforts towards high-performance devices based on PNCs, realising both devices with high efficiencies and stabilities through a single PNC processing strategy has remained a challenge. Herein, we demonstrate that diphenylpropylammonium (DPAI) surface ligands, found through a judicious ab initio based ligand search, provide a solution to this problem. This enhancement may also be attributed to the action of aromatic DPAm+ ligand: as DPAm+ is overall less flexible than long-chain OAm+/OA- ligands, substitution of the latter after DPAI treatment is also expected to result in denser packing of ligands and reduced degree of moisture penetration through the surface ligands, which is known to cause the phase transition to non-photoactive orthorhombic γ-CsPbI3. This speculation is confirmed with molecular dynamics (MD) simulations, which conclusively demonstrate that the diphenyl rings of DPAm+ are very effective in blocking moisture penetration into PNC lattice, while OAm+ shows presence of significant water concentration in the region occupied by surface ligands ; this enhanced encapsulating effect confers outstanding phase and performance stability for the SPLE-PNC devices.

Poster Presentation : **PHYS.P-223**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Unraveling the energetics of core-shell and alloy nanoclusters using machine learned moment tensor potentials

Hung Ngo manh, Sang Uck Lee[1,*]

Sungkyunkwan University, Korea
[1]*School of Chemical Engineering, Sungkyunkwan University, Korea*

The study of alloys system has been a topic of interest in materials science due to their unique properties and potential applications. In this work, we evaluate the formation energies and stability of various bulk alloys configurations and expand to the different nanocluster configurations. To address the challenge of accurately predicting the stability of alloys system, we employ the moment tensor potential (MTP) method, which has been shown to be a powerful tool for predicting the stability of alloys system. Using the MTP approach, we evaluate the formation energies and stability of various alloys at bulk and nanocluster systems considering core-shell and solid-solution configurations. The results provide valuable insights into the energetics and stability of these systems, and demonstrate the ability of the MTP method to accurately predict the stability of nanoclusters. Additionally, our study considers diverse range of configuration at different composition as well as the structure of nanoclusters in stability predictions, as different arrangements can have significant effects on the overall stability. Our findings have potential implications for the design and synthesis of novel nanomaterials and may provide a basis for future work in this field. Overall, this work showcases the potential of the moment tensor potential method in predicting the stability of nanoclusters, and provides valuable insights into the energetics and stability of transition metal nanoclusters.

Poster Presentation : **PHYS.P-224**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A SERS-based Galactose Sensor using Molecular Reporter-Immobilized Gold Nanoparticles

Eun Hae Heo, Hyejin Chang[1,*]

Division of Science Education, Kangwon National University, Korea

[1] *Division of science education, Kangwon National University, Korea*

Increased galactose levels in the blood and urine of newborns indicate galactosemia, and accumulation of galactose in the body can lead to liver disease, brain damage, and sometimes death. Therefore, it is necessary to develop a sensitive, fast, and reliable galactose diagnostic system that can enable early detection of galactose. In this presentation, we report a surface enhancement Raman scattering (SERS) based sensor using capillaries with advantages of sensitive, fast and simple detection. The SERS sensor was fabricated by decorating the inner wall of capillary with gold nanoparticles (Au NPs) and introducing 4-mercaptophenylboronic acid (4-MPBA) as molecular Raman reporter on the Au NPs. In our experimental design, 4-MPBA was converted to 4-mercaptophenol (4-MPhOH) by hydrogen peroxide (H_2O_2) produced from catalyzed reaction of galactose with galactose oxidase (GOx), and the reaction was observed through the SERS signal shifts. Through the optimization processes, selective galactose detection in the range of 0.01 to 50.0 mM was successfully achieved. These results indicate that the developed capillary SERS sensor has great potential for early diagnosis of galactosemia. Details of the results will be discussed in the presentation.

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Introduction of Distorted Cubes of $Sn_4I_4^{4+}$ in Zeolite Y for the Development of Zeolite-Based Phosphors

Hyeonseung Lim[*], **Hyeon Uk Choo**

Andong National University, Korea

Zeolites are well known host to encapsulate and stabilize nanoclusters and quantum dots. The complex tin iodide QDs were introduced in zeolite Y cavity to produce Sn,I,Cs,Na-Y with desirable luminescence properties. The composition, position and environments within the zeolite were learned by single-crystal crystallography using synchrotron X-radiation. Sn,I,Cs,Na-Y was prepared by allowing Cs,Na-Y to react with SnI_2 in a mixed organic solvent. It was refined in the space group Fd-3m (a = 24.873(2) Å) with all unique data to the final error indices R1 = 0.060 for the 1400 reflections for which $F_o > 4\sigma(F_o)$. Four Sn^{2+} ions and four I^- ions formed tetrahedrally distorted $Sn_4I_4^{4+}$ cubes. These cubes have 2.851(20) Å for Sn-I bond length and 106.4(10)˚ and 70.6(15)˚ for I-Sn-I and Sn-I-Sn angles, respectively. Each $Sn_4I_4^{4+}$ bonds to another I^- ion near the 12-rings and Cs^+ ions near the 4-rings, so that the cluster becomes $Cs_6Sn_4I_6^{8+}$. Then, each of core I^- of the cluster further bonds to Na^+ ion. Altogether, $[Na_4Cs_6Sn_4I_6]^{12+}$ clusters are formed in the supercages. These clusters form the $[Na_4Cs_6Sn_4I_6]^{12+}$ continuum by the bridging role of I^- ions on the plane of 12-rings. Partially hydrated Sn,I,Cs,Na−Y has a broad luminescence range from 400 to 800 nm, and through further hydration, the luminescence spectrum evolved with change of color from pale yellow to white.

Poster Presentation : **PHYS.P-226**

Physical Chemistry

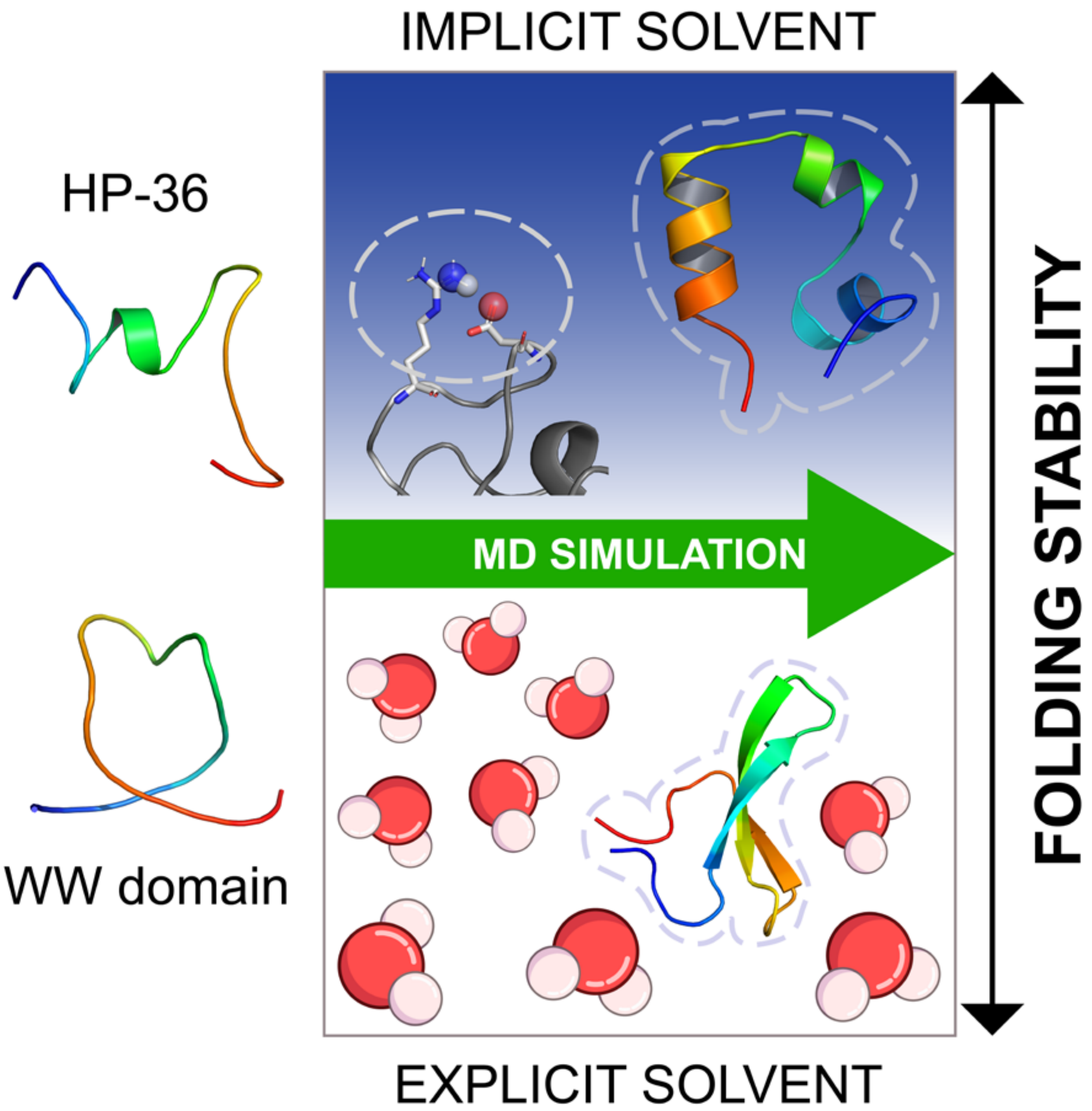
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Comparing the Influence of Explicit and Implicit Solvation Models on Site-Specific Thermodynamic Stability of Proteins

Myung Keun Cho, Song-ho Chong[1], Seokmin Shin[*]

Division of Chemistry, Seoul National University, Korea
[1]Faculty of Life Sciences, Kumamoto University, Japan

Understanding the molecular basis for protein stability requires a thermodynamic analysis of its folding. Thermodynamic analysis is often performed by sampling many atomistic conformations using molecular simulations that employ either explicit or implicit water models. However, it remains unclear to what extent thermodynamic results from different solvation models are reliable at the molecular level. Here, we quantify the influence of both solvation models on folding stability at the individual backbone and side-chain resolution. Using trajectories resulting from TIP3P explicit and generalized Born/surface area implicit solvent simulations of model proteins, we assess the residue-specific folding free energy components of a β-sheet protein and a helical protein. We found that the thermodynamic discrepancy from implicit solvent mostly originates from charged side chains, followed by the under-stabilized hydrophobic ones. In contrast, the backbone residue contributions in both proteins were comparable. Our study lays out the foundation to detailed thermodynamic assessment of solvent models in the context of protein simulation.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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

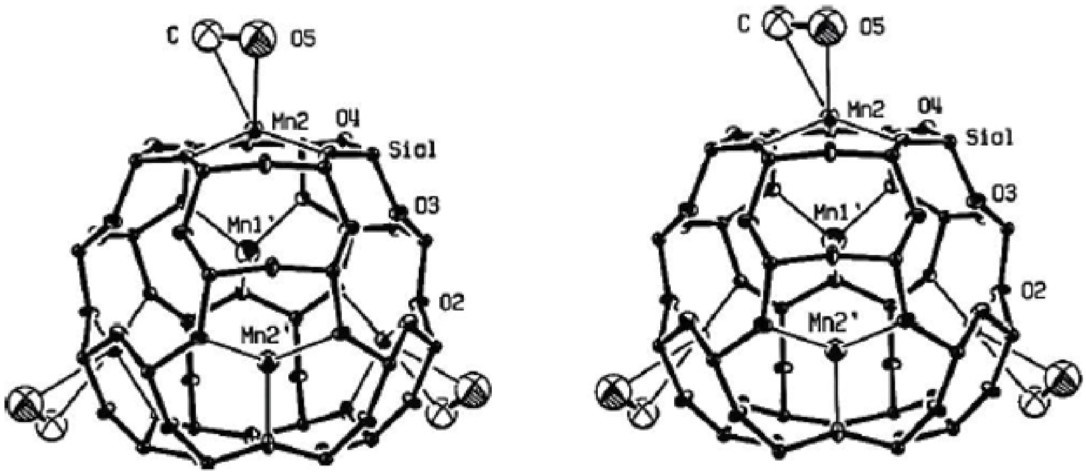
Poster Presentation : **PHYS.P-227**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation and Crystal Structure of Formaldehyde in the Fully Mn^{2+}-exchanged Zeolite Y (FAU, Si/Al = 1.56) by Direct Methanol Oxidation

Hyeonseung Lim, Hyeon Uk Choo, Woo Taik Lim[1,*]

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

The direct oxidation of methanol to formaldehyde was crystallographically observed within fully dehydrated, fully Mn^{2+}-exchanged zeolite Y by treating with methanol at 297(1) K, followed by evacuation. The structure of the formaldehyde complex of Mn^{2+}-exchanged zeolite Y was determined by single-crystal synchrotron X-ray diffraction techniques in the space group Fd-3m at 100(1) K . In this structure, the 37.5 Mn^{2+} ions are found at four crystallographic sites. 18 formaldehyde molecules per unit cell were all found opposite 6-rings in supercages, each coordinating to a site II Mn^{2+} ions. The formaldehyde molecules appear to be formed by oxidation of sorbed methanol molecules within zeolite Y cavities. The bond length of C = O in formaldehyde molecule is 1.399(20) Å. And the distances of Mn(2) to oxygen and carbon atoms of formaldehyde, 2.83(7) Å and 2.95(8) Å, respectively. From the relatively long distance between Mn^{2+} to formaldehyde, it may be seen that formaldehyde molecules are weakly bound to Mn^{2+} ions. The distances of carbon and oxygen of formaldehyde to the closest framework oxygens O(2) and O(4) are 3.23 Å and 3.49 Å, respectively which indicate hydrogen atoms interact with framework oxygens by van der Waals force.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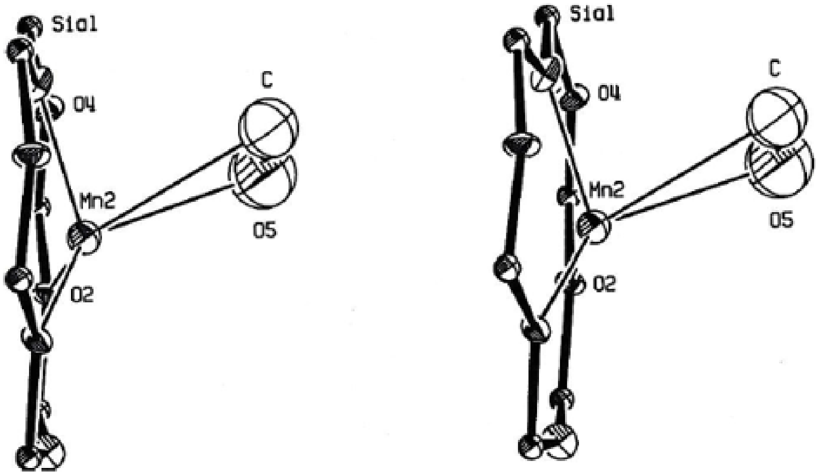
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Poster Presentation : **PHYS.P-228**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Intramolecular Charge Transfer Dynamics of Stilbazolium Derivatives by Time-Resolved Vibrational Spectroscopy

Jongwon Im, 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 where the charge transfers between the electron donor and acceptor groups often induce internal structural changes of chromophores, such as the rotation of the donor or acceptor group. For example, theoretical calculations, such as time-dependent density function theory method, have often suggested the twisted geometry of the electron donor group. However, experimental evidence for such structural changes with the ICT has rarely been reported, and the time-resolved electronic probe is fundamentally insensitive to these structural modifications of chromophores. In this work, we report the ICT dynamics of stilbazolium derivatives with or without the steric hindrance for the internal rotation of electron donor/acceptor groups. The *ortho*- and *para*-isomers of 4-N,N-diethylamino-N'-methylstilbazolium tosylate (DEST) appear quite similar in transient absorption (TA) measurements (time-resolved electronic probe), which shows that both isomers show apparent ICT dynamics in the excited states. On the other hand, femtosecond stimulated Raman measurements (time-resolved vibrational probe) reveal clear structural evidence of the ICT dynamics, especially in the vibrational frequency range of 1500-1650 cm^{-1}, where a *para*-isomer only shows the apparent internal rotation of the electron donor group (diethylaminophenyl) with the ICT in the excited states. Thus, the skeletal vibrational modes of styrylpyridinium backbone and similar pi-bridges, including the v_{8a} and $v_{C=C}$ modes, are suggested as one of the sensitive vibrational probes for the structural changes in the excited states.

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Poster Presentation : **PHYS.P-229**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Twisted Intramolecular Charge Transfer of Anthraquinone Derivatives in the Confined Environments of Reverse Micelles

Taehyung Jang, Sebok Lee, Jongwon Im, 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 in solar energy conversion, photovoltaics, fluorescence sensing, etc. Recently, we reported ultrafast (180 fs) ICT dynamics of 1-aminoanthraquinone (AAQ) by time-resolved Raman spectroscopy, where the major vibrational modes of $\nu_{C\text{-}N} + \delta_{CH}$ at 1200-1230 cm^{-1} and $\nu_{C=O}$ at 1300-1330 cm^{-1} represent the structural changes such as the internal rotation of the amino ($-NH_2$) group. The ICT dynamics of AAQ may depend on the local environments, such as the hydrogen bonding and microviscosity of solvent in the confined space of the reverse micelles (RMs). In this work, the photophysical properties and ICT dynamics of AAQs in the RMs have been investigated by steady-state and time-resolved electronic spectroscopy. Strong correlations between the ICT dynamics and several solvent properties (polarity, viscosity, hydrogen bonding, etc.) have been observed, which implies that the structural changes accompany the ICT of AAQ in the excited states. Understanding the photophysical properties of chromophores in heterogeneous microenvironments will be of great interest in many biological applications of these fluorophores.

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Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Spatial Charge Configuration Driven Exciton Dynamics in Electrochemically Doped InP Nanocrystals

Jumi Park, Dongho Kim[1,*]

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

Since semiconductor nanocrystals (NCs) hold strong promise for optoelectronic applications, there is an increasing demand for understanding charged NCs. Especially, deciphering the charge generation and subsequent recombination processes is of great importance to interpreting the device operation mechanism for functional device design and performance. Taking advantage of Solution-phase spectroelectrochemistry, a multi-response technique that obtains complementary information about electrochemical and spectroscopy, we can closely mimic device working conditions and demonstrate the characteristics of isolated NCs at that time.In this study, in situ spectroscopic changes in response to charging demonstrate the charge imbalance-driven exciton dynamics of tetrahedron- and tetrapod-shaped InP NCs. Absorbance responses under redox potential reveal that the charge injection efficiency of InP NC relies heavily on its geometric shapes. Even if tetrahedron and tetrapod have a similar size, the enlarged surface area of tetrapod-shaped structure brings efficient charge injection. Moreover, a tetrapod with branch lengths shorter than the negative trion Bohr radius of InP (LBranch < $r_{X\text{-}}B$) allows for strong suppression of nonradiative Auger recombination, thus almost maintaining photoluminescence intensity during charging. However, in the branch regime of LBranch > $r_{X\text{-}}B$, the photo-generated exciton of InP tetrapods exhibited higher Auger recombination rate constants than the former. Such indicates that a negative trion oriented linearly has large charge-exciton interaction energy and is prone to recombine nonradiative via Auger process. Our findings unearth a novel nanostructure as an attractive candidate for NC applications.

Poster Presentation : **PHYS.P-231**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Spectroscopic Elucidation on Exciton Dynamics of Perylene Bisimide Dye Assemblies in Solutions and Films

Seongsoo Kang, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

We have utilized time-resolved electronic and vibrational setups to explore the excited-state dynamics and vibrational coherence of one-dimensional perylene bisimide(PBI) H-aggregates in solution and film phases. In the solution phase, two PBI H-aggregates showcase the formation of the excimer state and the delocalized radical anion state in the excited state, respectively. Using femtosecond transient absorption (fs-TA) and time-resolved impulsive stimulated Raman scattering (TR-ISRS) measurements, we unveiled excited-state dynamics of PBI H-aggregates in two aspects: (1) the intermolecular interactions between PBI units in H-aggregates induce the formation of new excited states, excimer and delocalized radical anion states, and (2) the intermolecular out-of-plane along the aggregate axis and the PBI core C=C stretch Raman modes can be a crucial indicator to understand the coherent exciton dynamics in H-aggregates. Those excited-state Raman modes showed stationary peak positions during the excited-state dynamics. TR-ISRS analysis provides insights into the excited-state vibrational coherences concerning the excimer and charge-delocalized state formation in each aggregate system.Furthermore, we have been investigating how morphology affects the excited-state dynamics in films of PBI. We controlled how PBIs are packed in the solid state by changing the molecular structure of PBI. We anticipate this study will afford a better understanding of the impact of crystalline order on the excited-state dynamics and the impact different packing motifs have on the triplet state generation.

Poster Presentation : **PHYS.P-232**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Improve the thermal and electrical stability of organic glass film by controlled condition PVD method.

Taewoo Kim, Keewook Paeng[*]

Department of Chemistry, Sungkyunkwan University, Korea

Organic glasses are widely used for the organic electronics by having both mechanical properties of a crystal and the molecular disorder of a liquid. Limitations of the organic glass film which are the low conductivity and penetration of gases caused by the inefficient molecular packing. To cover up the limitations the more efficient the molecular packing and more dense film is required. Physical vapor deposition (PVD) method with controlled condition is known to make stable glass which has highly kinetic stability, is denser, and lower on the enthalpy landscape. Using the PVD method, we made 3-(dibenzo[c,h]acridin-7-yl)phenyl) diphenylphosphine oxide (TPPO-dibenzacridine) films by controlling the substrate temperature (T_{sub}) within the range of 0.80 T_g to 0.975 T_g. We found that the film made at T_{sub} = 0.90 T_g was up to 1.3% denser and had a fictive temperature (T_f) up to 50 K lower than the glass transition temperature (T_g). In addition, we investigated the relationship between the stability of the film and its electrical properties.

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Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Toward Recognition and Discrimination of his-tagged protein with lable-free Surface-Enhanced Raman Scattering

Dae Hong Jeong*, SungJun Kwak[1]

Department of Chemical Education, Seoul National University, Korea
[1]*Science Education, Seoul National University, Korea*

SERS is a spectroscopic technique that has the advantage of obtaining the intrinsic signal of a target samples. It is now easy to use various nanostructures to enhance the Raman signal of a target sample. The conventional methods of obtaining SERS signals by binding only molecules with thiol and amino groups to gold and silver nanostructures is no longer novel, and it is more important to obtain the signal of the desired target samples. Proteins are biopolymers composed of 20 amino acids and play a role in performing major biological functions such as enzymes, hormones, and antibodies in living organisms. There are many companies that use recombinant process to produce useful proteins. However, among the methods for analyzing proteins, electrophoresis requires a purification process, and ELISA has the difficulty of using antibodies that match the protein. In this study, we mimicked a method to capture proteins during the protein purification process and overcame the problems of the existing skills and perform high-speed analysis through SERS. We used coordination binding of histag tags expressed on recombinant proteins with metal cation and captured proteins by nitrilotriacetic acid (NTA) derivatives modified nanoparticles. Due to the size of the hotspot formed on the surface of the nanoparticles, we were able to obtain SERS signals for parts of the protein close to the histag. If the signals of different proteins can be acquired and distinguished in this way, our technique can contribute to the field of utilizing recombinant proteins.

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Poster Presentation : **PHYS.P-234**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Large-Area Symmetry-Broken $MoSe_2$ Synthesized by Flux-Controlled Chemical Vapor Deposition

JooHyeon Ahn, Youngdong Yoo[1,*]

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

Transition metal dichalcogenides (TMDCs) exhibit various novel electronic and optical properties depending on their structure. Monolayer TMDCs have been used for advanced 2D electronics and 2D optoelectronics due to their exceptional chemical and physical properties. Spiral TMDCs have been extensively utilized for novel nonlinear optics due to their broken symmetry. However, the selective synthesis of monolayer and spiral structure TMDCs is still challenging. Here, we report the selective synthesis of monolayer and spiral structure $MoSe_2$ using a flux-controlled chemical vapor deposition method. With a low flux, monolayer $MoSe_2$ is synthesized, whereas spiral $MoSe_2$ is obtained with a high flux. As-synthesized monolayer and spiral structure $MoSe_2$ are characterized by various techniques such as optical microscopy, atomic force microscopy, and Raman and photoluminescence spectroscopy.

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile synthesis of single-phase CrVO4 nanostructure for gas sensing

Yejin Kim, Myung Hwa Kim*

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

In terms of environment and safety, the detection of hazardous gases (NO2, H2, NH3, and CO) is important. For effective gas sensing, it is prerequisite for developing highly sensitive, selective, stable, and low-cost raw materials. Semiconductor metal oxide (SMO) such as chromium and vanadium oxide, has been widely studied as efficient gas sensor materials because of characteristic chemical and optical properties. In this work, thus, we report facile formation of single-phase CrVO4 nanostructure via simple acid-base reaction followed by thermal annealing process. Synthesized CrVO4 nanostructures were then characterized by using Field Emission Scanning Electron Microscope (FE-SEM), Energy Dispersive Spectroscopy (EDS), X-ray Diffraction (XRD), Transmission Electron Microscope (TEM). Further research will be conducted to confirm the gas sensing ability of CrVO4 nanostructures.

Poster Presentation : **PHYS.P-236**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication of high-efficiency P-N junction Hematite thin film for Hydrogen evolution reaction

Jae Hyun Park, Myung Jong Kang[1,*]

Gangneung-Wonju National University, Korea
[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

The production of Hydrogen through solar water splitting is one of the crucial electrochemical reaction. Hematite (α-Fe2O3) is a highly desirable semiconductor material for utilizing solar energy in photocatalysis due to its low cost, abundance, and broad light absorption spectrum, as well as its band gap of 1.9-2.2 eV. However, its poor conductivity is a significant drawback, which results from its short hole diffusion length, high electron-hole recombination rate, and brief minority carrier lifetime. Herein, we studied to compensate on the shortcoming of Hematite. The P-N junction, which has high efficiency and fast switching speed, was formed with n-type and p-type semiconductors. Hematite, a pristine N-type semiconductor, was mixed with Titanium to make a P-type semiconductor. To form a P-N junction on the doped electrode, Zinc, an N-type semiconductor, was doped, respectively. They were named ZX (X = Zn layer) according to the layer on which they were deposited. The deposited electrode was annealed at a high temperature. The fabricated thin film's surface was examined with SEM, while the elements' combination was scrutinized using XRD and XPS. Furthermore, a potentiostat was used to analyze the light efficiency of electrodes through LSV. The findings of these analyses confirmed the formation of the P-N junction and the subsequent increase in light efficiency.

Poster Presentation : **PHYS.P-237**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Utilization of Waste Melamine Resin into Photoelectrochemical Catalytic Electrode

Kyong suh Kim, Myung Jong Kang*

Department of Chemistry, Gangneung-Wonju National University, Korea

Melamine resin, formed by the copolymerization of melamine and formaldehyde, applied on various area in daily life like cookware, dishes, wood flooring, fibers due to useful properties of light weight, high temperature stability, excellence of durable and hardness. However, after-use waste melamine resin demands hundreds of years to decompose naturally, which causes serious environmental problem. Graphitic carbon nitride (g-C3N4) is well known photocatalyst material in research area because it is economic, eco-friendly, high stability and have proper band gap which can absorb visible-light region of solar light. Pristine g-C3N4 is synthesized by thermal treatment process of urea, melamine or dicyandiamide(DCDA). In this study, we introduce a method to fabricate catalytic electrode for photoelectrochemical reaction through utilization of waste melamine resin. Melamine resin added as supporting enhancer material during thermal treatment process to produce graphitic carbon nitride. The synthesized graphitic carbon nitride with melamine resin showed enhanced photocatalytic efficiency. This study suggests the way to synthesize highly efficient photo(electro)chemical catalytic electrode.

Poster Presentation : **PHYS.P-238**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile Fabricating Method of Mg-Al Layered Double Hydroxide Electrode for Photoelectrochemical Reaction

Yeonwoo Kim, Myung Jong Kang[1,*]

Department of chemistry, Gangneung-Wonju National University, Korea
[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Layered double hydroxide(LDH) which has plate-stacking structure, enables interlayer insertion of anions to compensate inter-plane positive charges. The characteristic structure of LDH enables various changes through negative ion exchange capacitance and possible changes in metal, negative ions, and preparation techniques, so that it regarded as attractive material which used for a various application. As the metal hydroxide layer and the anion are alternately arranged, it has a structure similar to that of Brucite, so it consists of a cation layer and an anion layer that can exchange ions between the layers. Various metal divalent and trivalent cations can be added, and various combinations of anions and cations are possible due to excessive cations, allowing the physical and chemical properties of the LDH nanostructure to be freely controlled. Herein, we studied on the way to utilize LDH materials as a photoelectrode. The Mg was used as divalent ions and Al was used for trivalent ions in synthesizing LDH structure, respectively. The optimal condition for fabricating electrode by synthesized MgAl LDH on FTO substrate was studied by changing temperature, density, device, etc.. The photocatalytic and electrochemical properties of fabricated electrodes was evaluated by measuring with LSV.

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Strategy on Improving Efficiency of BiVO4 Photoelectrode for HMF Oxidation Reaction

Serin Jung, Myung Jong Kang[1,*]

Gangneung-Wonju National University, Korea
[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Recently, plastic waste has increased a lot due to the impact of COVID-19. According to statistics, compared to 2019, food delivery increased by 76.8%, a courier by 20.2%, and plastic waste by 13.7%. Polyethylene terephthalate (PET), one of the petroleum-derived plastic, has the problem that it takes more than 150 years to decompose. To solve this problem, replacing PET into polyethylene furanoate (PEF), which takes only 40 years to decompose, has been studied widely. In addition, PEF has the advantage of minimizing the amount of carbon dioxide emissions. Due to these advantages, research on producing plastics from biomass is actively progressing. 5-hydroxymethylfurfural (HMF) is a substance derived from glucose through isomerization and dehydration reactions and has attracted a lot of attention because it can be converted into various added-value substances. After obtaining 2,5-furan dicarboxylic acid (FDCA) through oxidation of HMF, it is polymerized with ethylene glycol (EG) to obtain polymeric PEF. Bismuth Vanadate (BiVO4) is considered a suitable electrode to replace oxygen evolution reaction (OER) to HMF oxidation reaction by overcoming low reaction rate and high overpotential of pristine OER reaction. BiVO4 has emerged as a promising photoanode material due to its excellent chemical stability, eco-friendly material, and low cost. Therefore, herein, we studied on how to increase the reaction selectivity and efficiency of BiVO4 in HMF oxidation reaction

Poster Presentation : **PHYS.P-240**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mixed-Dimensional In-Plane Heterostructures Based on Monolayer MoS_2 and Dimension-, Composition-, and Phase-Controlled Mo/Te Compounds

Hyeonkyeong Kim, Youngdong Yoo[1,*]

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

Two-dimensional-other dimensional (0D, 1D, and 3D) mixed-dimensional heterostructures with novel properties have attracted attention in recent years. Here, we report a two-step chemical vapor deposition method for synthesizing mixed-dimensional in-plane heterostructures consisting of monolayer MoS_2 and low-dimensional Mo/Te compounds. The dimension, composition, and phase of Mo/Te compounds interfaced with MoS_2 are controlled by the Te flux. Mixed-dimensional in-plane 2D/2D/1D MoS_2/2H $MoTe_2$/Mo_6Te_6 heterostructures are synthesized under low Te flux conditions, whereas in-plane 2D/2D MoS_2/$MoTe_2$ heterostructures are obtained under high Te flux. This novel strategy for synthesizing mixed-dimensional in-plane heterostructures with atomically sharp interface will broaden the possibilities for the large-scale fabrication and applications of edge-contacted mixed-dimensional heterostructures.

Poster Presentation : **PHYS.P-241**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrochemical CO_2 reduction over Copper oxide based nanowire

Ho seong Yang, Juyoung Maeng, Youngku Sohn*, Choong Kyun Rhee

Department of Chemistry, Chungnam National University, Korea

In this study, we investigated the improved activity of copper oxide nanowires deposited with gold (Au) for the electrochemical CO_2 reduction reaction. Although copper oxide nanowires are widely used for electrochemical CO_2 reduction reaction due to their high conductivity, stability, and catalytic activity, their efficiency still needs improvement. We confirmed the synthesis and characteristics of Au-deposited copper oxide nanowires through SEM, XRD, and XPS analysis, and measured their activity for CO_2 reduction reaction using electrochemical and photocatalytic methods. As a result, we found that Au-deposited copper oxide nanowires showed significantly enhanced activity for electrochemical CO_2 reduction reaction compared to normal copper oxide nanowires. Products were measured using gas chromatography, and the main products include carbon oxide and hydrogen.

Poster Presentation : **PHYS.P-242**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 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

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. The IR ion-dip and IR-UV double resonance spectra revealed that H+Phe-Ala-Ala ions were present in at least two different conformers in the ion trap. 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 were 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-243**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Dual enhancement effect of SERS via graphene quantum dots decorated silver nanoshells

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Advanced Raman enhancement platforms using plasmonic nanoparticles (NPs) and graphene quantum dots (GQDs) named ‘dual enhancement’ platforms have drawn attention. The dual enhancement platform is expected to have various advantages from combining the two SERS enhancement mechanisms, charge-transfer induced chemical mechanism (CM) of GQDs, and electromagnetic mechanism of plasmonic nanoparticles. In this study, solid-support substrates were designed based on bumpy silver nanoshells (Ag NSs) and GQDs to figure out how to maximize the SERS efficacy of our system as a dual enhancement platform. GQDs with armchair and zigzag edge structures were applied and the different optical properties and electronic structure of the two kinds of GQDs were expected to affect the characteristics of CM enhancement. Rhodamine 6G and Rhodamine B were used as probe molecules to compare the dual-SERS effect between two types of substrates. Dual-SERS substrates showed different performances depending on the laser. Depending on the type of laser or substrate, the ratio of Raman signal increase of rhodamine 6G was found to be different for each band and this ratio was compared. Especially R6G Raman band-related xanthene ring and phenyl ring increased the Raman signal at different rates.

Poster Presentation : **PHYS.P-244**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effects of Methylation on Morphology of DNA: Computer Simulation Studies

<u>Janghee Hong</u>, Rakwoo Chang*

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In carcinogenesis, preneoplastic cells transform into tumor cells, grow into carcinoma, and are eventually metastasized to other organs via blood vessels. The metastasized tumor cells can grow back in the metastasized organ to cause tumors [1]. Many studies have reported that the methylation of the 5th carbon in the cytosine residues in CpG islands of DNA in human cancer cells may be closely related to the cancer and that the demethylation of 5-methylcytosine may be used as a cancer therapy [2,3]. However, how the methylated cytosine in CpG islands would affect normal DNA to cause cancer has not been studied extensively up to now. In this study, the molecular dynamics simulation was used to study DNA conformational changes according to the degree of methylation in the cytosine residues in a CpG island. We mimic the CpG island with 16 base pairs that only consist of C and G nucleic acids. Then, we randomly methylated cytosine residues. We report the effects of methylation on structural properties such as H-bonding distance, DNA curvature, and tortuosity.References[1] Delpu, Y.; Cordelier, P.; Cho, W. C.; Torrisani, J. DNA Methylation and Cancer Diagnosis. Int. J. Mol. Sci. 2013, 14 (7), 15029–15058.[2] Pfeifer, G. P.; Xiong, W.; Hahn, M. A.; Jin, S.-G. The Role of 5-Hydroxymethylcytosine in Human Cancer. Cell Tissue Res. 2014, 356 (3), 631–641.[3] Szyf, M. The Role of DNA Hypermethylation and Demethylation in Cancer and Cancer Therapy. Curr. Oncol. 2008, 15 (2), 72–75.

Poster Presentation : **PHYS.P-245**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular Dynamics of Simulation studies: Structural Insights into FOX Transcription Factors with DNA

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The histone H1 protein is one of the five major histone proteins. unlike other histone proteins, H1 proteins do not form the nucleosome 'Core DNA'. Instead, instead, the histone H1 protein binds to the DNA surrounding the core DNA and fixed it in place. our study found FOXA protein, a pioneer factor that can replace this histone H1 protein. The FOXA1 factor replaces linker histone H1 by regulating DNA bending. Experimentally, it was confirmed that the transcription activation was different when the types of proteins were different, and the wing2 part of the proteins confirmed that the DNA-protein interaction affected the transcription activity. With this result, we've run simulations on different DNA + protein complexes (including DNA-FOXA1, DNA-FOXD3, DNA-FOXC2, and DNA-FOXA1-wing2), and calculated each RMSD, RMSF, and contact-map. and the CURVES+ software program was used for the values related to curvature.Reference[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.

Poster Presentation : **PHYS.P-246**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mechanism of dramatic slowdown of crystallization rate at doped binary glass system

Tae Young Jin, Keewook Paeng*

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Crystalline organic materials have a disadvantage derived from crystal boundary and untidy crystal grains. To solve this disadvantage, researchers composed organic materials in an amorphous state. Thus, an amorphous organic material is not limited by the orientation of its molecules. However, a pure amorphous material has a new disadvantage that crystallization proceeds. To eliminate the new disadvantage, we chose doping as a method to slow down the crystallization rate. At an electron transport layer among the components of organic light-emitting diodes, the mobility of electrons is an important performance. Bathophenanthroline (BPhen) has very high electron mobility among organic materials, but it has a fast crystallization rate. To slow down the crystallization rate of BPhen, we doped 8-quinolinolatolithium (Liq) from 0 to 17 volume% as physical vapor deposition. We measured the crystallization rate at a specific temperature in the range of 30-150℃ as home-built polarized microscope. As the doping concentration increased, the crystallization rate started to slow down rapidly. When doping at 17 volume%, the crystallization did not proceed at all. The first factor of the rapid slowdown of crystallization rate is kinetic due to the rise in glass transition temperature (T_g). When the plotting data as crystallization rate – T/T_g, high concentration case have an additionally lower crystallization rate. Thus, there is an additional factor increasing T_g. The second factor is dynamic, unlike the first which is kinetic. Therefore, in the dramatic slowdown of the crystallization rate by doping, both kinetic and dynamic factors act simultaneously.

Poster Presentation : **PHYS.P-247**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigation of Electronic coupling in Imine Molecule-Bridged Zinc oxo cluster Dimer Systems

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

Zinc oxide is a promising electrode material for lithium-ion batteries due to its abundance in nature, affordability, and high theoretical capacity (987 $mAhg^{-1}$). However, it has low electrical conductivity and requires significant improvement due to its volume expansion problem during lithium absorption. In previous research, we confirmed performance improvement using π-conjugated molecule-bridged silicon quantum dot clusters with alkyne bonds for silicon anode materials that have similar issues. In order to prevent volume expansion issues, we propose the construction of a giant cluster connected by π-conjugated molecule-bridges with imine bonds, using tetranuclear carboxylate zinc oxo clusters (ZOC) as building blocks. Imine bond is dynamic covalent bond, which and has reversible and self-healing properties, which can prevent cluster isolation caused by the volume expansion of ZOC. However, an important property for use as a lithium ion anode material is electrical conductivity. To assess the potential of imine molecule-bridged ZOC anode materials, we calculated the electronic coupling of imine bridged ZOC dimer and compared with alkyne bridged ZOC. The ZOC dimer linked by an imine bond has an electronic bond value of $8.60x10^{-7}$ eV, while the alkyne bond is $8.08x10^{-8}$ eV. Imine bonds can act as excellent cluster bridging molecules due to their electrically conductive and self-healing properties.

Poster Presentation : **PHYS.P-248**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Shape-Dependent Diffusion Dynamics of Nanoparticles in Solvent-Swollen Entangled Polymer Networks Probed by Single Particle Tracking

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Understanding nanoparticle dynamics in polymeric systems is an essential step for a variety of applications including filtration, particle dispersion in composites, and drug delivery to name a few. Lately, research efforts have focused on the shape dependency of nanoparticle diffusion dynamics to show those rod-shaped particles exhibit a higher diffusivity than spheres of similar size in biological matrices such as mucus and agarose spheroids. In this study, we investigate the effect of particle anisotropy on translational diffusion through unentangled and entangled polymer networks. Gold nanorods (GNRs) with a diameter × length of 15 × 85 nm and gold nanospheres (GNSs) with a diameter of 28 nm were used. These gold nanoparticles (GNPs) bore similarity in hydrodynamic diameter and were labeled with Cy3 dyes for single-particle tracking via wide-field fluorescence microscopy. Thin films of poly(methyl methacrylate) PMMA (M_e = 9.2-13.8 kg/mol) with M_w = 7.2 and 98.5 kg/mol containing GNPs at a picomolar concentration were swollen with solvent vapors of chloroform ($\chi = -0.80$). At several swelling ratios, movies were recorded to track the nanoscale motion of individual GNPs. From statistical assessment of single particle trajectory, mean-squared displacement, van Hove correlation function, and non-Gaussian parameter, we compare the diffusivity and anomaly of the diffusion dynamics of GNRs and GNSs.

Poster Presentation : **PHYS.P-249**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Pyridinium-Substituted Halogenated BODIPY Dyes for Mitochondria-Targeted NIR Fluorescence Cell Imaging and Photodynamic Therapy

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Photodynamic therapy (PDT) in combination with cell imaging-based diagnosis, in other words, imaging-guided PDT (IgPDT) is an attractive cancer treatment modality. As part of ongoing efforts to develop fluorescent triplet photosensitizers (PSs) for clinical use in IgPDT, herein we report the synthesis and spectroscopic, theoretical, and in vitro characterization of pyridinium-substituted halogenated boron dipyrromethene (BODIPY) dyes (PyBXI, X = H, M, Br). We revealed that the incorporation of cationic pyridinium, styryl moieties, and triethylene glycol chains on the innate BODIPY structure enabled the resultant PyBXI dyes to display desirable properties, including mitochondria-targeting ability, absorption and fluorescence within the phototherapeutic window (650–850 nm), and water solubility. The pyridinium group facilitated the formation of charge transfer (CT) states, which, instead of mediating triplet state formation as proposed previously, resulted in unfavorable nonradiative decay processes. Nevertheless, the halogenation enhanced the intersystem crossing, rendering PyBMI and PyBBrI to exhibit improved singlet oxygen generation capabilities compared to that for PyBHI. In vitro experiments revealed that PyBBrI dyes exhibited a mitochondria-targeting ability, which may have facilitated their accumulation in the cancer cells and NIR fluorescence for cell imaging. Furthermore, PyBBrI dyes showed a high photocytotoxicity, with half maximal inhibitory concentration (IC50) values of 96 nM and 219 nM for MCF-7 and HeLa cells, respectively. Overall, we have successfully shown the synthesis and characterization of BODIPY-based theragnostic agents, which may contribute to developing strategies for the design of novel PSs applicable to practical cancer treatment.

Poster Presentation : **PHYS.P-250**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigating the Photodissociation Dynamics of CF_2BrCF_2I in CCl_4 through Femtosecond Time-ResolvedInfrared Spectroscopy

Seongchul Park, JuHyang Shin, Manho Lim[*]

Department of Chemistry, Pusan National University, Korea

The photodissociation dynamics of CF2BrCF2I in CCl4 at 280 ± 2 K were investigated by probing the C−F stretching mode from 300 fs to 10 μs after excitation at 267 nm using time-resolved infrared spectroscopy. The excitation led to the dissociation of I or Br atoms within 300 fs, producing the CF2BrCF2 or CF2ICF2 radicals, respectively. All nascent CF2ICF2 underwent further dissociation of I, producing CF2CF2 with a time constant of 56 ± 5 ns. All nascent g-CF2BrCF2 isomerized into the more stable a-CF2BrCF2 with a time constant of 47 ± 5 ps. Furthermore, a-CF2BrCF2 underwent a bimolecular reaction with either itself (producing CF2BrCF2Br and CF2CF2) or Br in the CCl4 solution (producing CF2BrCF2Br) at a diffusion-limited rate. The secondary dissociation of Br from a-CF2BrCF2 was significantly slow to compete with the bimolecular reactions. Overall, approximately half of the excited CF2BrCF2I at 267 nm produced CF2BrCF2Br, whereas the other half produced CF2CF2. The excess energies in the nascent radicals were thermalized much faster than the secondary dissociation of I from CF2ICF2 and the observed bimolecular reactions, implying that the secondary reactions proceeded under thermal conditions. This study further demonstrates that structure- sensitive time-resolved infrared spectroscopy can be used to study various reaction dynamics in solution in real time.

Poster Presentation : **PHYS.P-251**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The Dynamics of Bimolecular Proton Transfer in Aqueous Solution Probed by Time-resolved Infrared Spectroscopy

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The neutralization of an acid by a base is one of the fundamental reactions in solutions. We observed aqueous bimolecular proton transfer, using a photoacid, 8-hydroxy-1,3,6-trisulfonate-pyrene (Pyranine, PyOH), which reacts with azide (N_3^-) as a strong acid when electronically excited. The most significant IR spectra changes of PyOD between electronic ground-state and excited-state occur in the spectral region of 1400-1650 cm^{-1}. Azide has a strong band at 2042 cm^{-1} and its conjugated acid (DN_3) at 2133 cm^{-1}. Time-resolved vibrational spectra were measured in these spectral regions after excitation of PyOH in the presence of N_3^- in D_2O solution with a 400-nm pulse. In the presence of low base concentration (< 150 mM of N_3^-), the dominant reaction path was found to be the bimolecular reaction between the base molecule and deuteron (D^+) which was dissociated from the excited state PyOD, rather than direct reaction from acid-base complexes that was observed in high base concentration. The bimolecular reaction involved in acid-base reaction observed via this research will be presented.

Poster Presentation : **PHYS.P-252**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Optimal Fluorescence Enhancement of Bioimaging Dyes on Composite Silver Nanosurfaces

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

Metal-enhanced fluorescence (MEF) has drawn considerable attention in various fields, such as biological and chemical sciences, due to the improvements in photostability and brightness of fluorescent dyes. The enhanced emission has been explained by increased absorption and radiative relaxation rates of dyes due to the strong local electric field and plasmon-coupled emission of metal nanoparticles induced by surface plasmon resonance (SPR), respectively. Furthermore, the spectral overlap of dye's emission with dipole (DSPR) or quadrupole SPR (QSPR) has been reported as one of the critical factors for strong MEF. We have recently reported strong MEF of dyes with the combined SPRs of DSPR and QSPR of composite nanostructures. This study investigates optimal fluorescence enhancements of Alexa Fluor dyes with composite silver colloidal films (SCFs) composed of small and large silver nanoparticles. Alexa Fluor dyes are widely used in in vivo bioimaging due to their selective binding capability to active sites and high photostability in spite of low quantum yields in an aqueous solution. First, the particle diameters of silver nanoparticles for efficient DSPR and QSPR have been determined. Then, the combination of the DSPR and QSPR of small and large nanoparticles has been sought for optimal fluorescence enhancements. The emission kinetics in time-correlated single-photon counting measurements and the local field enlargements by the finite-difference time-domain simulations have been added to reveal fluorescence enhancements of Alexa Fluor dyes.

Poster Presentation : **PHYS.P-253**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Dye-assisted transmittance enhancement of Mie resonanator based optical nanofilters

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Compared to their plasmonic counterparts, Mie resonator-based optical systems are able to sustain strong resonances at small spatial scales and be relatively free from optical loss. In this work, we introduce a Mie-resonance based method to enhance the transmission efficiency of transmissive optical nanofilters. We integrate quantum emitters inside a previously described PMMA-Ag core-shell nanowire system that acts as an efficient dipole resonator when excited by light polarized parallel to the nanowire. This hybrid resonator system can theoretically achieve 30 percent more transmission at resonance compared to the original resonator, all while retaining comparably high resolution.

Poster Presentation : **PHYS.P-254**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photoisomersim and dissociation dynamics of S-nitroso-mercaptoethanol (MceSNO) probed by femtosecond IR spectroscopy

Hojeong Yoon, Seongchul Park, Manho Lim[*]

Department of Chemistry, Pusan National University, Korea

S-nitroso-mercaptoethanol (MceSNO) has been used as a NO donor or transporter in biological systems, but its photochemical applications have not been fully explored because of its lack of photodynamics. To investigate the photoexcitation dynamics of MceSNO in water, femtosecond time-resolved infrared spectroscopy was used to measure dissociation, recombination, and linkage isomerization after photoexcitation at 320 nm. Metal-ON linkage isomers were found between transition metals and NO, and similarly, sulfur-ON linkage isomers (MceSON) were found at room temperature. After 320 nm photoexcitation, 5% of the MceSNO molecules underwent linkage isomerization, returning to MceSNO over a barrier in 400 ps. The reaction rate was affected by temperature, and the energy of the barrier was determined to be 3.90 kcal/mol. Additionally, 48% of the dissociated radical species recombined, and the remaining 43% underwent a bimolecular reaction with surrounding MceSNO to form disulfide MceSSMce, generating additional NO. These findings provide insights into the photochemistry of MceSNO and its potential applications in various fields.

Poster Presentation : **PHYS.P-255**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of a Local Charge State Fixation Method for Calculating Reorganization Energy in Molecule-Bridged Silicon Quantum Dot Dimer Systems

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

In order to calculate the reorganization energy required for electron (or hole) hopping in a dimer system where the donor and acceptor are bridged by a molecule, it is necessary to have the geometry and force constants of the system in which the charge is localized in the donor or acceptor. However, since these states are not ground states, the optimization process is difficult. To address this issue, we have developed a method called Local Charge State Fixation (LCSF) to calculate the reorganization energy required for electron (or hole) hopping in molecule-bridged silicon quantum dot (Si QD) dimer systems. LCSF involves replacing the donor or acceptor of a neutral state dimer with a donor or acceptor of a charged state monomer, while fixing and grafting the internal geometry and force constants of the charged state donor or acceptor. We performed geometry optimization and force constant matrix calculation of both neutral state dimers and charged state donors/acceptors using the Gaussian 16 package with the DFT/B3LYP method and 6-31G(d,p) basis set. The matrices of the grafted systems were generated using MATLAB, and the reorganization energies between grafted systems were calculated through normal mode analysis. We used Si QDs with a diameter of 0.83 nm ($Si_{35}H_{35}$) as the donor and acceptor, and various bridging molecules including polyethylene (PE), polyacetylene (PA), oligoyne (OY), p-divinylbenzene (VPV), 1,2-Bis(4-vinylphenyl)ethyne (VPEPV), and 1,4-bis(4-ethenylphenylethynyl)benzene (VPEPEPV).

Poster Presentation : **PHYS.P-256**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Thermal Conductivity Calculation of Molecule-Bridged Silicon Quantum Dot Dimer Systems Using Atomistic Green's Function Method

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Using the atomistic Green's function (AGF) method, we calculated the thermal conductivity of various molecule bridges in silicon quantum dot (Si QD) dimer systems at different temperatures (T=0 K~1000 K). The molecular bridges we selected were polyethylene (PE), polyacetylene (PA), oligoyne (OY), p-divinylbenzene (VPV), 1,2-bis(4-vinylphenyl)ethyne (VPEPV), and 1,4-bis(4-ethenylphenylethynyl)benzene (VPEPEPV). Si QDs with a diameter of 0.83 nm ($Si_{35}H_{35}$) were used for the contacts. We performed geometry optimization and force constant matrix calculation of the Si QD dimer systems using the Gaussian 16 package with the DFT/B3LYP method and 6-31G(d,p) basis set. The AGF method was implemented using MATLAB R2018b code. As expected, we found that longer bridging molecules resulted in lower thermal conductivity. Among the vinyl-phenyl series bridging molecules, the thermal conductivity was lower than that of the polyethylene and oligoyne series, but higher than that of the polyacetylene series. In general, the thermal conductivities of the PA bridge systems were the lowest. Based on these results, we suggest using PA as a molecular bridge to improve the thermoelectric performance of thermoelectric materials made with Si QDs.

Poster Presentation : **PHYS.P-257**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigation of organic ligand and annealing temperature dependence of electron mobility and electronic structure of indium oxide nanocrystals thin films using thin film transistor devices and electrochemical measurements

Quang Trung Le, Hyeok Yun, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

The electronic structure of indium oxide (In_2O_3) nanocrystals (NCs) capped with oleic acid (OA), benzoic acid (BA), or 4-aminobenzoic acid (4ABA) was studied as a function of annealing temperature (T_{Ann}). The NCs were deposited on SiO_2/Si wafers for electron mobility measurements, and T_{Ann} was varied from 150 to 350℃. At T_{Ann} = 200℃, BA-capped In_2O_3 exhibited higher electron mobility compared to 4ABA-capped In_2O_3 due to their ability to interact via π-π stacking. However, as the temperature increased to T_{Ann} = 250 ℃, resulting in higher electron mobility of 4ABA-capped In_2O_3 due to the formation of N=N bonds between the remaining ligands, confirmed by Raman spectroscopy. At T_{Ann} = 250℃, the reorganization energy of BA- or 4ABA-capped In_2O_3 NCs was very similar, indicating that the ligands had decomposed almost completely, confirmed by infrared spectroscopy and thermogravimetric analysis. The electronic structure was studied by cyclic voltammetry and energy-resolved electrochemical impedance spectroscopy after annealing the NCs on ITO electrodes at T_{Ann} = 150℃, 200℃, or 250℃. The valence band peak was observed near -6.8 V for the BA- or 4ABA-capped In_2O_3 NCs films at T_{Ann} =150℃ or 200℃, but not at T_{Ann} =250℃. For the OA-capped In_2O_3 NCs, the peak near -6.8 V was always observed, indicating that it was formed by the electronic interaction between the In_2O_3 NC and the carboxylate group of the ligands.

Poster Presentation : **PHYS.P-258**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nonlinear Optical Imaging of Few-Layer Hexagonal Boron Nitride

Yeri Lee, Juseung Oh[1], Hyeon Suk Shin[2], Sunmin Ryu[*]

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Due to its broad bandgap (~6 eV), hexagonal boron nitride (hBN) has recently attracted considerable attention for its nanophotonic applications in the UV range. High-resolution methods like TEM and STM have been widely used to analyze the structure of the synthesized hBN. As they are limited to very small length scales, effective techniques are required to characterize crystalline domains and defects in synthesized wafer-scale hBN of high quality. [1] In this study, we report on two correlated nonlinear optical scanning methods to characterize the structure of hBN on a larger dimension: second-harmonic generation (SHG) and two-photon photoluminescence (PL). Two types of few-layer hBN samples were prepared by mechanical exfoliation and chemical vapor deposition (CVD). CVD-grown hBN samples showed substantially weaker SHG but stronger visible PL signals than exfoliated ones. Grain boundaries of polycrystalline CVD-hBN were revealed with polarized SHG imaging. Also, the linear correlation of orientation distribution and Raman width of various hBN crystals implies the potential for nonlinear optical scanning to be used as a new structural indicator for synthesized hBN film.Since the properties of hBN films are governed by their structure, the reported method will contribute to the controlled synthesis of hBN with specific material properties. [2][1] K. Y. Ma, et al., Nature 606.7912 (2022): 88-93.[2] Y. R. Lee, et al., in preparation

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **PHYS.P-259**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Charge-Transfer Absorption Band in Two-Dimensional PTCDA/MoS2 Heterocrystals

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Poster Presentation : **PHYS.P-260**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tetrahydroxy-Tetramethyl-Cyclotetrasiloxane as a High Sensitivity EUV and E-Beam Resist for Next-Generation Lithography Applications

Jiyoung Bang, Hyeok Yun[1], Wonchul Kee[1], Hyun-Dam Jeong[1,*]

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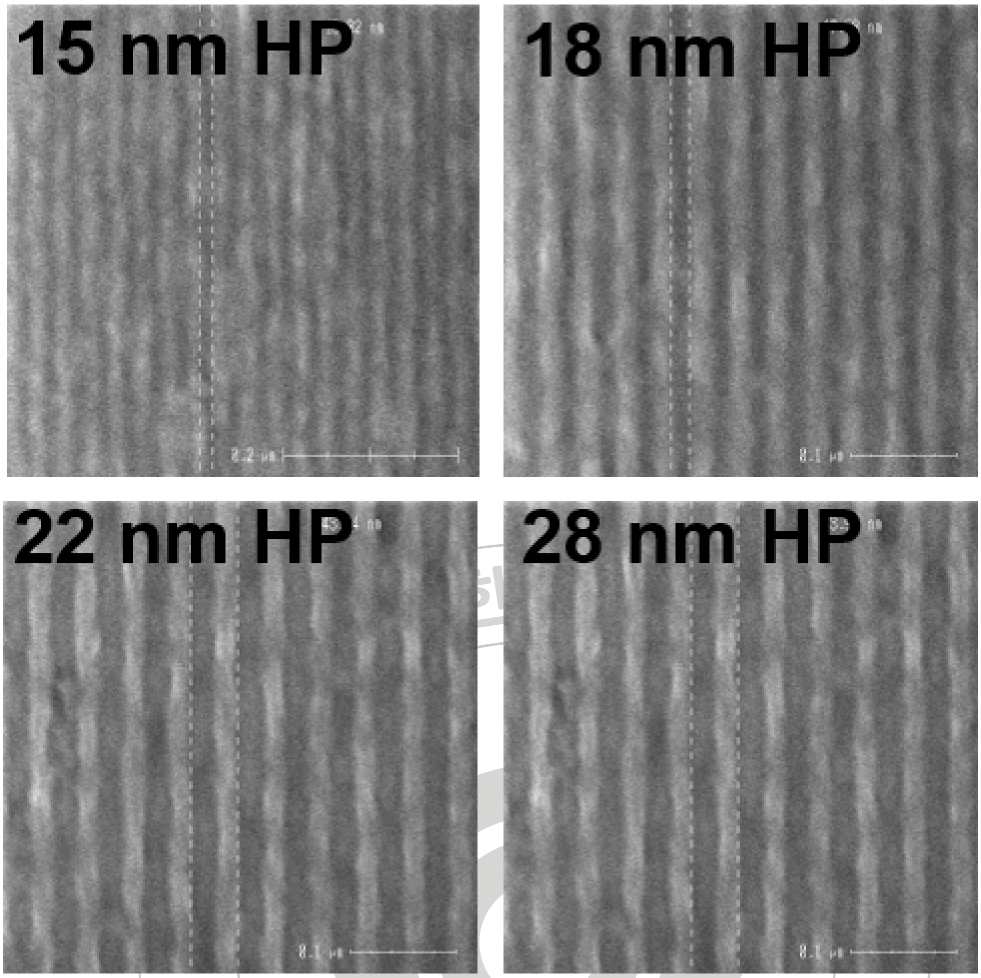
Extreme ultraviolet lithography (EUVL) has become the leading lithography technology in semiconductor manufacturing. The development of an effective EUV resist has been one of the key achievements enabling this success. Inorganic resists have attracted considerable attention for next-generation EUVL applications due to their high mechanical strength and dry etch resistance. In this study, tetrahydroxy-tetramethyl-cyclotetrasiloxane (tetraol) was utilized as an EUV and e-beam resist. And it had an electron beam sensitivity(D_{50}) of 21.9 uC/cm^{-1} and an EUV absorption coefficient of 9.89 cm^{-1}. In EUVL, the photoresist film was formed 22nm HP pattern at 55mJ/cm^2. Also it have shown etch resistance that is 1.7 times higher than that of bottom anti-reflective coating (BARC) and 65.4 times times higher than that of spin on carbon (SOC). To find the reason why tetraol has higher sensitivity despite having a lower EUV absorption coefficient than tin oxo cluster, the electron beam exposure area was analyzed through FT-IR, TOF-SIMS, and XPS. Tetraol's four hydroxy groups contribute in part to its high sensitivity. The hydroxyl groups can form network siloxane bonds by thermal energy and electron beams, allowing them to act as negative-tone photoresists. They can also form hydrogen-bonded aggregates, enabling the production of thin films. Additionally, we confirmed that various radicals were generated and involved in the reaction during the electron beam exposure.


15 nm HP
18 nm HP
22 nm HP
28 nm HP

Poster Presentation : **PHYS.P-261**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Novel Approach for Calculating Electron Transport in Constant Current Mode in π-Conjugated Molecular Bridged Si QD Dimer for Lithium Ion Batteries

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In previous study, we evaluated the influence of cross-linked structure manipulation on the electrochemical performance of anode materials based on π-conjugated molecular bridged silicon quantum dot (Si QD) clusters (SQCs). As a result, we found that the SQC with the highest specific capacity among the three SQCs was dependent on the applied current density. To understand this result, we developed a novel approach to estimate electron transport across molecular bridges in constant-current mode, called the "constant-current-mode transport computational method", based on the non-equilibrium Green's function method combined with the discrete-state Gaussian expansion. Electron transport in constant current mode is a process in which high-energy electrons enter the outermost Si QD and then transfer to neighboring Si QDs to diffuse and lithiate into the entire SQC. Herein, Note that these Si QDs are in equilibrium due to Li+ cations. We performed the calculation by substituting the increase in the number of electrons entering the Si QD with the increase in electron density. Remarkably, we observed that the electron transport behavior obtained by increasing the number of electrons injected into the Si QDs was analogous to the specific capacity of the experimental SQCs.

Poster Presentation : **PHYS.P-262**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Comparative theoretical study of numerical wave-packet propagation, MCTDH, and surface hopping methods on coupled-bidirectional photo-dissociation dynamics of the PCET of FHCl

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Numerical nuclear wave-packet propagation, multi-configuration time-dependent Hartree (MCTDH) of nuclear wave-packet, and semi-classical surface-hopping (SH) are well-established theoretical methods for studying quantum aspects of nuclear behaviors in molecular systems. Though many previous studies comparing these methods, the comparative studies on the dynamics with intimately coupled dissociative pathways are still quite limited. The proton-coupled electron transfer (PCET) process of the charge-transfer excited state of FHCl is one of the most delicate and complicated cases because two dissociation channels corresponding to proton transfer (PT) and electron transfer (ET) are bi-directionally coupled through non-adiabatically interacting three electronic states. We recently reported the early-time dynamics of PCET process in FHCl by the numerical wavepacket propagation method, showing that the ratio of PT product (F + HCl) is higher than that of ET (FH + Cl) with branching ratio χ = PT/(PT+ET) = 0.67. The same photo-dissociation dynamics are studied again in the present work with MCTDH and SH methods implemented in SHARC package. Results by the three different methods will be compared and discussed in this presentation. The knowledge from this work will be applied to more complicated systems with higher dimensionality such as NH_3Cl (DOF = 9).

Poster Presentation : **PHYS.P-263**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Structural and Rotational Effects of Antimicrobial Peptides on Membrane Insertion and Disruption

Inhyeok Choi, Yeonho Song[1], Hyonseok Hwang*

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

In this study, we used molecular dynamics (MD) simulations and potential of mean force (PMF) calculation to examine the structural and rotational effects of antimicrobial peptides (AMP) on the membrane insertion and disruption. Two types of AMPs were selected to see the variation of structure and free energy of AMPs depending on the residue alteration. PMF calculations reveal that the nonpolar facet of the two peptides is flipped upside down as a peptide permeates into the center of membranes. Flipping of the AMPs is observed at the membrane interface for both AMPs and appears to be a substantial process for AMP insertions. MD simulation analysis also shows that flipping occurs more easily in LK-L8P that has a proline residue substituted for leucine. As a result, proline plays an important role in AMP insertions into the membrane by assisting the flipping process.

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Poster Presentation : **PHYS.P-264**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular dynamics simulation study of the role of membrane cholesterols in cancer drug resistance

Namho Kim, Hyonseok Hwang[1,*]

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

In this study we investigated the effect of membrane cholesterols (CHOL) on doxorubicin (DOX) permeating through normal and cancer membranes using all-atom molecular dynamics (AA-MD) simulations and potential of mean force (PMF) calculations. Normal cell, sensitive and resistant cancer cell membranes were modeled by increasing the ratio of CHOL in symmetrized POPC bilayers. In the PMF profiles for DOX permeation, the highest energy barrier is observed in the resistant cancer cell model while free energy wells are found in the normal cell membrane model and the sensitive cancer cell model displays an energy barrier in between. Subsequent thermodynamic integration (TI) decomposition analysis reveals that although increase in the number of membrane CHOL reduces unfavorable interactions between DOX and lipid molecules, favorable interactions of DOX with water are much more dominant in the normal cell model than the other models. In addition, it is also found that DOX induced membrane deformations at the bilayer surface in normal cell model system cause water molecules to penetrate even into the center of the lipid bilayer, but it rarely occurs in the resistant cancer model system where the high concentration of CHOL makes membranes much rigid. The hydrated DOX inside the normal membrane model leads to acyl chain rearrangement to diminish energy barriers to cross the lipid bilayer. Therefore, reducing membrane CHOL concentration could be a potential strategy to avoid drug resistance in cancer cells.

Poster Presentation : **PHYS.P-265**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photoluminescence Study of Mechanically Exfoliated 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. We were able to obtain and characterize 2D picene crystals as thin as 15 nm using atomic force microscopy. Upon excitation at 360 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. We will discuss the possible role of each process and explore experimental methods to distinguish between them.

Poster Presentation : **PHYS.P-266**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Distinct Behavior of Sodium Lauryl Ether Sulfate penetrating into the Normal and Atopic Skins: *in silico* Approach

Yeonho Song, Hyonseok Hwang[1,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Department of Chemistry, Kangwon National University, Korea*

Sodium lauryl ether sulfate (SLES) is an anionic surfactant that is widely used in our daily products. In this study, we examined the energetic behavior of a SLES monomer permeating into the normal and atopic skins using molecular dynamics simulations combined with potential of mean force (PMF) calculations. The normal and atopic skins are modeled and represented by varying the ratio of skin components such as ceramide, cholesterol, and fatty acids. The resulting PMF profiles demonstrate that a SLES surfactant permeates into the atopic skin more easily than into the normal skin because the anionic surfactant prefers cholesterol-rich regions which are found more in the atopic skin. Constant force-steered MD (cf-SMD) simulations are also conducted to assess the surfactant transfer from SLES micelles to the skin bilayer. The regression analysis from the cf-SMD trajectories also indicates that surfactants in the micelle migrates into the atopic skin more easily and faster than into the normal skin.

Poster Presentation : **PHYS.P-267**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Optimal Stimulated Raman Excited Fluorescence Obtained by Tuning Independently

Taesu Kim, Sang-Hee Shim[1,*]

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

Stimulated Raman excited fluorescence (SREF) is a new hybrid spectroscopy that combines high chemical specificity of Raman scattering with superb sensitivity of fluorescence detection. Even though SREF demonstrated far-field single-molecule vibrational spectroscopy for the first time, the single-molecule signal is much lower than those from directly excited fluorophores due to the low detection efficiency and low quantum yield of infrared fluorophores. SREF of visible dyes failed to achieve single-molecule sensitivity due to lack of proper light source for fulfilling all the requirements for vibrational resonance, electronic pre-resonance and suppression of one-photon excitation. In this study, we use two optical parametric oscillators (OPOs) synchronously pumped by a common pump source at 1031.2 nm. This laser system can generate two independently tunable pulses in 640-1150 nm for optimizing the wavelengths of pump and Stokes beams for efficient vibrational excitation by stimulated Raman scattering (SRS) as well as subsequent pumping to the electronic excited state. We first set the frequencies of the pump (wp) and Stokes (ws) that fulfilled the conditions for electronic pre-resonance (i.e. wabs = wp +(wp - ws)) and vibrational resonance (wp - ws = wc=c) where wabs is the absorption maximum and wc=c is the vibrational frequency of the C=C skeletal mode. From there, we obtained optical SREF signals at various wavelength by changing the pump while maintaining wp-ws . We measure the SREF spectra of various visible fluorophores with this strategey. We anticipate that our scheme for SREF of visible dyes significantly increases the sensitivity of SREF to make single-molecule vibrational spectroscopy as a practical means for overcoming the spectral limit of single-molecule fluorescence spectroscopy.

Poster Presentation : **PHYS.P-268**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Novel Tin-Hybridized Cyclosiloxane material for EUV Photoresist

Soyeong Heo, Hyun-Dam Jeong[1,*]

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

Poster Presentation : **PHYS.P-269**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Resonant Raman Scattering of PTCDA multilayers on Graphene

Kyungtaek Oh, Eunbeen Jeon, Sunmin Ryu*

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

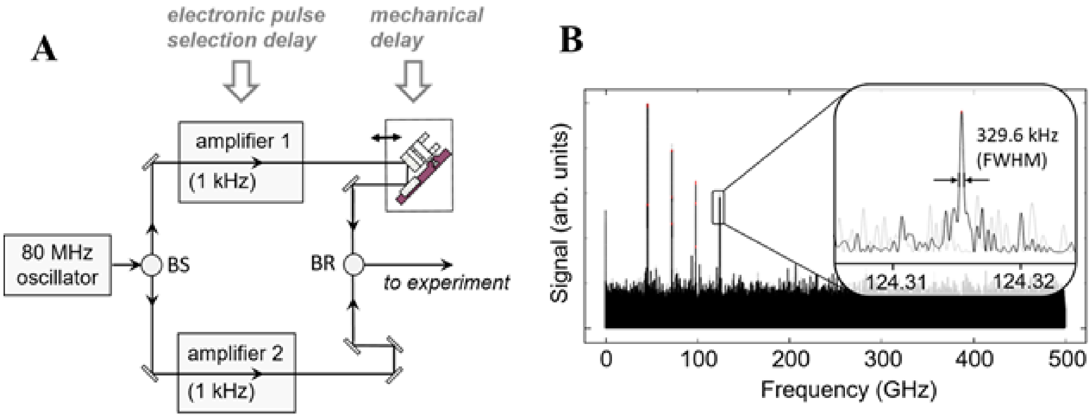
Poster Presentation : **PHYS.P-270**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular Beam Spectroscopy with an Infinite Interferometer: Spectroscopic Resolution and Accuracy

In Heo, Schultz Thomas[1,*]

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

CRASY stands for Correlated Rotational Alignment Spectroscopy and is a multi-dimensional spectroscopic technique that combines rotational spectroscopy and mass spectrometry. It provides mass-selected high-resolution rotational Raman spectra of samples. The experiment is based on two laser pulses (alignment and ionization) and a molecular beam that interact in a time-of-flight mass spectrometer. The IR alignment laser pulse rotationally excited molecules and created a coherent rotational wave packet. The UV probe laser pulse ionized these molecules and probed the coherent wave packet. The resulting cations were collected by an MCP detector. By scanning the time delay between alignment and probe laser pulses, we measured a time-dependent signal modulation based on molecular rotation. This time-domain signal modulations were Fourier-transformed to frequency domain spectra for each mass channel.In our experiment, the limit of the spectral resolution was determined by the range of time delay between two pulses like interferometry. We selected two techniques, mechanical delay, and electronic delay. The laser oscillator is 80 MHz and the distance with the neighbor pulse is 12.5 ns. The opto-mechanical delay line adds a 4.8 m delay (corresponding to 16 ns). The electronic pulse-selection delay adds discrete delays in multiples of 12.5 ns.Pulse selection from a stable laser oscillator allows to perform interferometric spectroscopy with an effectively infinite interferometer. This approach removes the dominant resolution limitation for interferometric measurements and allows us to obtain the world’s highest-resolution scanned interferometric data. Herein, we present mass-correlated rotational Raman spectra with sub-kHz effective resolution over a 500 GHz spectral range. The achieved resolution is several orders of magnitude better than that achieved by any preceding rotational coherence spectroscopy or Fourier-transform IR spectroscopy measurements and corresponds to the scanning of km-scale path differences.


A
electronic pulse selection delay
mechanical delay
amplifier 1
(1 kHz)
80 MHz oscillator
BS
BR
to experiment
amplifier 2
(1 kHz)
B
Signal (arb. units)
329.6 kHz (FWHM)
124.31
124.32
0
100
200
300
400
500
Frequency (GHz)

Poster Presentation : **PHYS.P-271**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

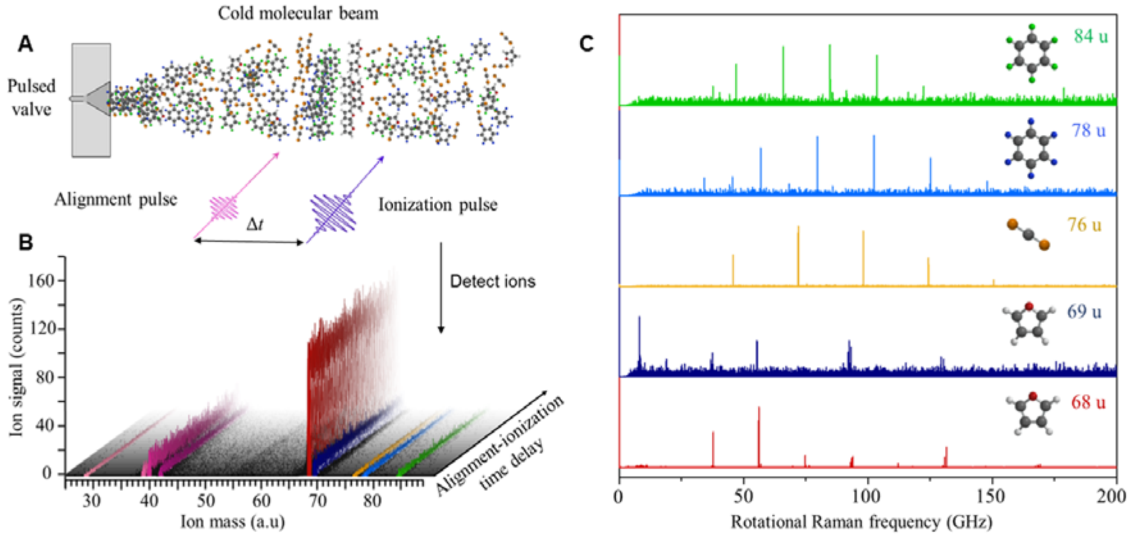
Studying Heterogeneous Molecular Samples by Correlated Laser Spectroscopy

Begum Rukiye Ozer, Schultz Thomas[1,*]

PhD. student, Ulsan National Institute of Science and Technology, Turkey

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

Would it not be nice if signals for each component in a heterogeneous sample could be ‘marked’ and sorted using a single spectroscopic measurement, without any prior purification? Correlated rotational alignment spectroscopy (CRASY) is a multi-dimensional laser technique that correlates rotational Raman spectroscopy to mass spectrometry. This study shows that we can mark each species in a heterogeneous sample by rotational spectra and sort them out by their ion mass. Herein, we resolved 12 different spectra in a mixture of furan, 13C-furan, carbon disulfide, benzene and perdeuterated benzene with a single measurement. This capability of CRASY circumvented a long-standing problem of traditional spectroscopic techniques requiring pure samples, where purification is often expensive and time-consuming, or sometimes impossible.



Poster Presentation : **PHYS.P-272**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and Characterization of Tin-Hybridized HSQ for EUV Photoresist

Minyeop Kim, Jiyoung Bang[1], Hyun-Dam Jeong[2,*]

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

Hydrogen silsesquioxane (HSQ), a negative tone photoresist widely used for e-beam lithography, is expected to show excellent performance in EUV lithography as well. Specifically, HSQ is advantageous for ultrafine patterns because of its inherent structure, exhibiting line edge roughness (LER) of less than 2nm. However, HSQ has a disadvantage in EUV sensitivity because the main element of HSQ, Si, has a low optical absorption cross section at 92 eV. To overcome this limitation, we have substituted some of the Si atoms in HSQ with Sn atoms, which have a high EUV optical absorption cross section, and named it CNU-TOC-05. The structure of CNU-TOC-05 was confirmed by FT-IR, DLS, and XPS, and it was also confirmed to be a negative tone photoresist through e-beam lithography. CNU-TOC-05 is expected to form EUV photoresist patterns with excellent resolution and sensitivity due to its significantly improved EUV sensitivity compared to conventional HSQ.

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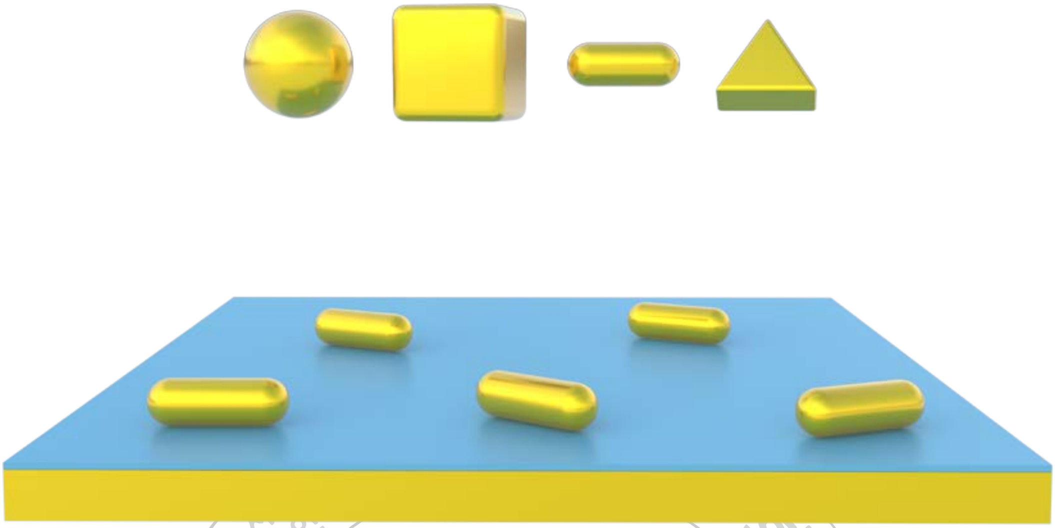
Poster Presentation : **PHYS.P-273**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Influence of Gold Nanoparticle Shapes on Plasmon-Driven Reaction Yields

Seokheon Kim, Sangwoon Yoon[1,*]

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

The field of plasmonics began to grow explosively in the early 2000s and is still growing steadily on account of fascinating beneficial properties for applications like photovoltaics, photocatalysis, and high-performance sensor. With the explosive growth of plasmonics, development of novel metal nanostructures and theoretical research have been made, but effect of gold nanoparticle morphology on hot charge carrier generation efficiency is still under debate. In this study, we aim to investigate the relationship between hot charge carrier generation efficiency and nanoparticle morphology using the nanoparticle-on-mirror (NPoM) system with four different shapes: spherical (AuNSs), cubic (AuNCs), cylindrical (AuNRs) and triangular gold nanoparticles (AuNTs). We compared decarboxylation of 4-MBA between gold nanoparticle (AuNP) and Au-film reaction which are well known as plasmon driven reaction at 633 nm and 785 nm each and among them, AuNR which are known as absorbing material, shows the highest reactivity in both wavelengths. This investigation strong evidence of hot charge carrier generation relates to absorption of gold nanomaterials. We expect our work could inform the design of more efficient plasmonic devices and technologies.



Poster Presentation : **PHYS.P-274**

Physical Chemistry

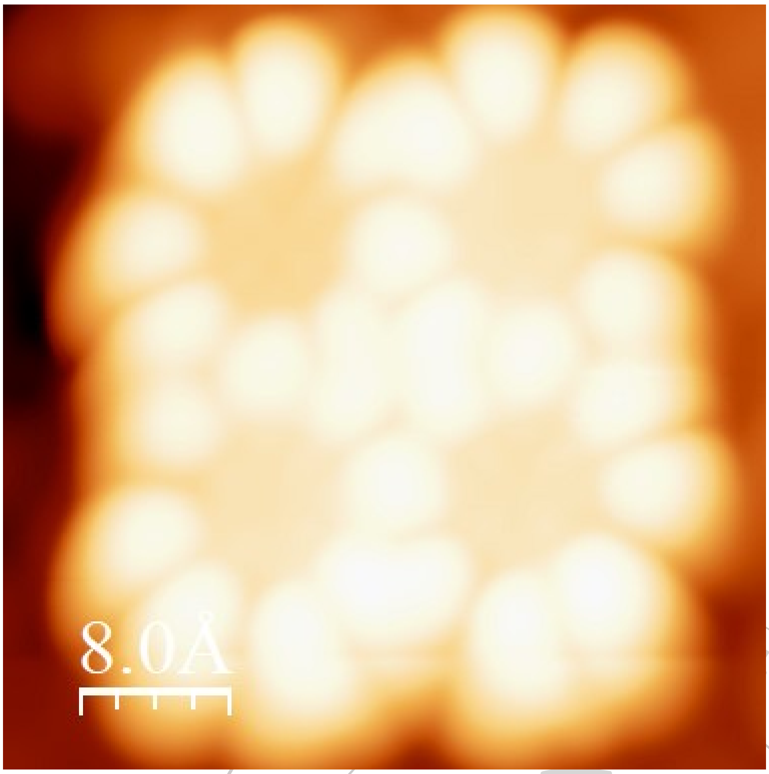
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Lanthanide double-decker complexes as on-surface quantum nanomagnets

Luciano Colazzo

Center for Quantum Nanoscience, Ewha Womans University, Korea

Lanthanide based Single-molecule magnets are promising materials for future spintronic applications, such as ultra-high-density memory devices, quantum computing, sensing and information processing units.Using a variety of methods, we have succeeded in synthesizing and purifying different double-decker phthalocyanine complexes (MPc2; M = Y, Er, Tb, among others). We deposited them onto metal substrates in ultra-high vacuum (UHV) for scanning tunneling microscopy/spectroscopy (STM/STS) investigations. Terbium double-deckers have recently been the object of several investigations on quantum spin control within molecular spin transistor and several STM settings. Departing from these former investigations, we focused our attention on ErPc2 as the magnetic properties of the Erbium molecular complex have not been carefully characterized yet. ErPc2 and TbPc2 are expected to display different magnetic properties that can be accessed with STMs and several other techniques, within our reach. This study describes the magnetic and electronic characterization of Erbium double-decker supported on a Au(111) substrate. Single molecular units were investigated via STM and STS in order to extract structural, electronic and magnetic properties. We observed Kondo effect on the ErPc2 scaffolds, indicative of the presence of an unpaired electron on the molecular complex. Such electron can be potentially exploited as a sensor for the quantum control of the electronic and nuclear spins of the enclosed and well isolated Er atom.


8.0Å

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Poster Presentation : **PHYS.P-275**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Defect Characterization Based on the Analysis of Nitrogen Adsorption on UiO-66 with Machine Learning Approach

Yu Chen, Yongchul Chung*

School of Chemical Engineering, Pusan National University, Korea

Adsorption isotherms provide valuable insights into defect characterization of nanoporous materials such as metal-organic frameworks (MOFs). However, conventional Grand Canonical Monte Carlo (GCMC) simulations are often computationally intensive for materials with large pores or defects. This study presents an alternative approach to defect characterization of UiO-66, a well-known MOF in defect engineering field, based on the analysis of saturation loading (SL) and BET surface area (BETSA) obtained from the N_2 adsorption isotherms predicted by machine learning (ML) model. Our developed ML model demonstrates high accuracy in predicting N_2 adsorption isotherms, thereby enabling more efficient determination of SL and BETSA. This study showcases the potential of ML techniques for accurate and efficient characterization and defect identification of nanoporous materials based on adsorption isotherms

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Poster Presentation : **PHYS.P-276**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

segmental dynamics of miscible blend of low-molecular weight glass formers and polymer

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

Segment dynamics of polymers, the related dynamics of glass transitions, can be investigated by analyzing the rotation of fluorescent molecules in the polymer matrix via an image-rotating fluorescence correlation microscope. Basic research on solvent-induced glass transition through polymer solutions or blends, such as those frequently used in batteries or PR, is insufficient.Therefore, in order to measure the rotational dynamics of the binary mixture near Tg, the rotational dynamics near Tg was measured by using pPDI as the probe and adjusting the blend concentration using low molecular weight glass-former OTP(o-terphenyl) and 1,3,5-Tris(naphthyl)benzene(TNB) heterogeneous mixture and polystyrene, Poly(methyl methacrylate)(PMMA). Through this, the temperature dependence of polymer solution dynamics and the shape of the correlation decay can be calculated.

Poster Presentation : **PHYS.P-277**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Anisotropic Plasmon Coupling in Au Nanorod-Au Nanosphere Assemblies

Seokhyun Yun[*], **Sangwoon Yoon**[1,*]

Chung-Ang University, Korea

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

Gold nanoparticles (AuNPs) have numerous applications, including as sensors, biological imaging agents, surface-enhanced Raman scattering (SERS) substrates, catalysts, and photothermal therapy agents. Among them, gold nanorods (AuNRs) are anisotropic nanoparticles with plasmon modes in two different directions: transverse and longitudinal. This characteristic can be further extended by attaching gold nanospheres (AuNSs) to the AuNR to create an assembly (AuNR@AuNS). In this study, we successfully synthesized AuNR@AuNS nanoassemblies and investigated plasmon coupling at both the ensemble and single-nanoassembly level. Our results show that both the transverse and longitudinal modes of AuNRs shift to longer wavelengths when AuNSs are attached to the side and end of the AuNRs. Using dark-field single-particle scattering spectroscopy, we further demonstrate that this plasmon coupling is strongly dependent on the polarization of the excitation light. Our findings pave the way for site-specific control of molecules in nanogaps between AuNRs and AuNSs.

Poster Presentation : **PHYS.P-278**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ultrafast Excited-state Aromatization in 1,6-methano[10]annulene

Jinseok Kim

Department of Chemistry, Yonsei University, Korea

Baird's rule of reversed aromaticity in the T1 state and its extension to the excited singlet (S1) state have been verified only by theoretical and computational methods until recently. We suggested effective experimental spectroscopic tools that provide direct evidence of the excited state aromaticity. In particular, the vibrational analysis critically supported the aromaticity reversal in the S1 state instead of quantum calculations due to computational difficulties in the excited singlet (Sn) state.Tovar, Casado, and co-workers reported the synthesis of TMTQ molecule, which is a 1,6-methano[10]annulene (M10A) co-oligomer with thiophene and dicyanomethylene units on both sides of core M10A moiety. A significantly small ΔEST gap was observed in TMTQ and the T1 state stabilization by Baird's rule was proposed to account for this phenomenon.According to this perspective, we demonstrated the aromatization of TMTQ in the excited state induced by an intramolecular CT process via electronic and vibrational spectroscopic analysis. Steady-state absorption and fs-transient absorption (fs-TA) spectroscopic measurements in solvents of varied polarity were carried out to identify the intramolecular CT process, followed by time-resolved IR (TRIR) and quantum calculations to confirm the excited state aromatization accompanied by the structural reorganization of the nonaromatic core M10A unit.

Poster Presentation : **PHYS.P-279**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The chemical fluctuation theorem governing gene expression, protein maturation and annihilation.

Jin Hyung Kim, Ji-Hyun Kim, Jaeyoung Sung[*]

Department of Chemistry, Chung-Ang University, Korea

Fluorescent proteins are effective tools for quantifying gene expression dynamics in living cells. While it is known that these proteins emit fluorescence upon undergoing maturation processes, the impact of these processes on protein levels measurable by fluorescent proteins remains unclear. Here, we propose a new version of the chemical fluctuation theorem (CFT) that applies to proteins with general gene expression and maturation dynamics and can be used to analyze experimental observables such as the mean and variance of matured protein levels in living cells. We also explore how dynamic cell-to-cell fluctuations in gene expression dynamics and non-exponential lifetime distributions of proteins can affect these observables. This research provides a reliable and quantitative understanding of gene expression and protein maturation dynamics in living cells.

Poster Presentation : **PHYS.P-280**

Physical Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Predicting Association and Dissociation Rates in Protein-DNA Interactions: Insights from a Theoretical Model

Jingyu Kang, Ji-Hyun Kim[1,*], Jaeyoung Sung[1,*]

Chung-Ang University, Korea

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

We have developed a model to predict the association and dissociation rates of protein-DNA binding, which are essential for accessing genetic information. Our research involved testing this model on thousands of different lacoperator sequences. Our findings suggest that the efficiency of the protein in recognizing different targets is correlated with the lifetime of the protein-DNA complex. We used such correlations to predict the randomness of association and dissociation times. Our study offers insights into the mechanisms underlying protein-DNA interactions and provides a theoretical framework for predicting and understanding protein-DNA binding.

Poster Presentation : **PHYS.P-281**
Physical Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tin Monoxide-Based Resist for EUV Lithography

Wonchul Kee, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

We synthesized tin monoxide photoresist named as TIMO-SA. The E-beam sensitivity of the TIMO-SA thin film was measured using acetic acid as a solvent where it was developed at TMAH (Tetramethylammonium hydroxide) 2.38 wt% for 30 seconds. As a result, it was confirmed that D50 as 6 μC/cm2 and contrast as 3.79. However, it confirmed that TIMO-SA using acetic acid as a solvent was not dissolve in a developer solution even in a wide area other than the expose portion when exposed to extreme ultraviolet rays. In order to solve this problem, it was decided to find a condition in which the development time after electron beam exposure, was 10 seconds or less. E-beam sensitivity of the TIMO-SA thin film using ethyl lactate as a solvent was investigated, where the film was developed for 10 seconds using TMAH 0.0238 wt% as a developer. As a result, D50 and contrast is confirm each 22.88 μC/cm2 and 2.30. In this case, unlike TIMO-SA using acetic acid as a solvent, the phenomenon was not found, and electron beam lithography is plan to be attempted at National Nanofab Center.

Poster Presentation : **ANAL.P-72**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

In-situ Spectroelectrochemical Analysis of Formamidinium Lead Iodide Perovskite Quantum Dots for Tracking their Degradation

Hyoin Kim, Taeyeon Kim[1], Seog Joon Yoon[2], Donghoon Han[*]

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

Multi-dimensional ABX3 hybrid perovskites have emerged as one of the key ingredients to be applied in many fields. Various forms of perovskites (dot, nanorod, platelet, bulk layer structure, etc.) are utilized by regulating the growth to depend on specific dimensions. Understanding the photoinduced charge carrier dynamics of perovskite quantum dots (PQDs) under electrochemical reactions can be a significant factor in applying perovskite quantum dots to solar-driven chemistry and optoelectronic devices. In this study, the reaction products were identified through cyclic voltammetry, X-ray photoemission spectroscopy, in-situ UV/Vis absorption spectroscopy, and detailed conversion reaction mechanisms of lead iodide perovskite quantum dot form were studied under electrochemical reactions. Comprehensive characterization identified irreversible oxidation transformation mechanisms for PQDs. This study can provide deep insight into the electrochemical behavior of PQDs for the successful application of solar-driven chemistry and optoelectronic devices.

Poster Presentation : **ANAL.P-73**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A Fully Integrated, Microfabricated Analytical System for On-Chip Detection Based on Indium Tin Oxide Interdigitated Array Electrodes

Hyeri Jeon, Je Hyun Bae[1], Donghoon Han*

Department of Chemistry, The Catholic University of Korea, Korea
[1]*Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, Korea*

A new strategy for the fabrication of a three-electrode system used in microchip systems is described herein. A standard photolithography method was used to fabricate an on-chip, integrated, three-electrode system with a solid-state reference electrode, an indium tin oxide (ITO) interdigitated array (IDA) working electrode, and an electrodeposited Pt counter electrode. Electroplating conditions, such as the potential and time, were investigated with respect to the stability and uniformity of the electrodeposited films. A solid-state reference electrode was fabricated using an electropolymerized poly-1,3-phenylenediamine (poly-m-PD) layer on a nanoporous Pt surface. The electrochemical performance of the three-electrode system was evaluated using cyclic voltammetry. The experimental results demonstrated that the proposed system could work as a solid-state reference electrode that can be integrated into microchips for miniaturized analytical systems.

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Poster Presentation : **ANAL.P-74**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ionization behaviors of RDX and PETN in atmospheric pressure chemical ionization

He-Ryun Choi, Sung-Seen Choi[1,*]

Sejong University, Korea

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

1,3,5-Trinitro-1,3,5-triazine (RDX) and pentaerythritol tetranitrate (PETN) are widely used explosives along with 2,4,6-trinitrotoluene (TNT). RDX is a nitramine (N-NO_2) explosive, and PETN is classified as a nitrate ester (R-O-NO_2) one. In general, they are analyzed by high performance liquid chromatography (HPLC) and gas chromatography (GC). For HPLC analysis, detection limits of RDX and PETN are about 5 and 10 ng, respectively, when using UV detector, while the detection limits are improved by using mass spectrometry (MS) detector. In atmospheric pressure chemical ionization (APCI), RDX produces mainly $[RDX + NO_2 - H]^-$ and $[RDX + NO_2]^-$, while $[PETN - H]^-$ and $[PETN + NO_3]^-$ are detected as the product ions of PETN. By adding chloride dopant, chlorinated molecule, $[M + Cl]^-$, is formed. In this study, RDX and PETN were directly analyzed using APCI-MS without separation, and difference in the ionization behaviors with the solvent systems was investigated. When RDX and PETN were mixed, $[RDX + NO_3]^-$ was newly produced by the transfer of NO_3^- from PETN. Chemical structures and energies of the product ions were calculated to explain the experimental results.

Poster Presentation : **ANAL.P-75**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Tuning Plasmonic Properties by Thiol in 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*

Mesoporous Silica Coated Gold Nanorods (AuNR@mSiO_2) was investigated with mercury amalgam and thiolation to study the plasmon effect of the AuNR@mSiO_2 during the reaction with mercury and thiol AuNR@mSiO2. In this work, we first incubation nanoparticles using mercury and LSPR peak of single-particle was study using dark-field microscopy and spectroscopy. Then, LSPR peak of the AuNR@mSiO_2 showing blue shifting and broadening in the linewidth as present from previous study. Interestingly, the peak was going to red shifting after the solution was changed into thiol and narrowing in they LSPR. To check the influence of the thiol, variant carbon length was using for this study. The peak become narrower due to the increase of the carbon length. This condition giving promising study to study the plasmon behavior of the AuNR@mSiO_2 and can be using for many applications, such as drug delivery and sensor.

Poster Presentation : **ANAL.P-76**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Influence of oxygen plasma treatment on the electrocatalytic activity of AuNRs immobilized on ITO surfaces

Mukunthan Ramasamy, Ji Won Ha[1,*]

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

Surface plasmon resonance (SPR) is a unique property associated with certain metallic nanomaterials (e.g., Au, Ag, Cu). The localized surface plasmon resonance (LSPR) is a collective oscillation of conduction band free electrons in metallic nanostructures due to interactions with light. The LSPR property of metallic nanoparticles has attracted great attention for many applications that include photocatalysis and electrocatalysis. The LSPR spectrum of plasmonic nanoparticles is influenced by the size, shape, composition, and change in refractive index (RI) of the surrounding medium. Anisotropic gold nanoparticles (AuNRs) have broadly tunable size, shape, and structure-dependent optical properties, and have good photostability and biocompatibility. Oxygen plasma is a partially ionized gas consisting of electrons, ions, and neutral atoms/ molecules. Radiofrequency (RF) plasma, a nonthermal plasma is often used to remove surface capping material and to change the morphology of metallic nanoparticles (NPs). In this study, single gold nanorods (AuNRs) of considerable size were immobilized on the ITO surface and exposed to oxygen plasma. We discuss the spectral, structural changes, and electrocatalytic activity of oxygen plasma exposed AuNRs by dark-field (DF) microscopy and spectroscopy, scanning electron microscopy (SEM), and cyclic voltammetry (CV). We address the plasmonic effect on AuNRs and the potential-dependent catalytic activity of plasma-treated AuNRs at the single-particle level.

Poster Presentation : **ANAL.P-77**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Machine learning (ML) liquid chromatography retention time prediction model augments the dansylation strategy for metabolite analysis of urine samples.

Eun Woo Choi, Han Bin Oh[*]

Department of Chemistry, Sogang University, Korea

Herein, a standalone software equipped with a graphic user interface (GUI) is developed to predict liquid chromatography mass spectrometry (LC–MS) retention times (RTs) of dansylated metabolites. Dansylation metabolomics strategy developed by Li et al. narrows down a vast chemical space of metabolites into the metabolites containing amines and phenolic hydroxyls. Combined with differential isotope labeling, e.g., 12C-reagent labeled individual samples spiked with a 13C-reagent labeled reference or pooled sample, LC–MS analysis of the dansylated samples enables accurate relative quantification of all labeled metabolites. Herein, the liquid chromatography RTs for dansylated metabolites are predicted using an artificial neural network (ANN) machine-learning model. For the ANN modeling, 315 dansylated urine metabolites obtained from the DnsID database are used. This RT-prediction model is embedded into a user-friendly GUI and can be used for identifying nontargeted dansylated metabolites with unknown RTs, along with accurate mass measurements. Hereby, we can identify Dansylated metabolite in spite of shortage of MS/MS information. Furthermore, the developed software can help identify metabolites from a urine sample of an anonymous healthy pregnant woman.

Poster Presentation : **ANAL.P-78**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

An Image-Based Deep Learning Approach for Predicting Essential Mechanical Properties of Hydrogels

Jumi Kang, Kyueui Lee*

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Hydrogels have significant potential as scaffolds in tissue engineering, and their mechanical properties, such as modulus and viscosity, must be tailored to the intended application. Therefore, predicting the mechanical properties is critical for developing effective hydrogel-based biomaterials. However, conventional mechanical testers like rheometers are costly, time-consuming, and require expertise in rheology. To address this challenge, we developed an image-based deep learning model that can predict essential mechanical properties, including viscosity, density, rigidity, and porosity, of hydrogels by simply analyzing SEM images. Specifically, we applied a Convolutional Neural Network (CNN) to extract relevant features from the input data and used an unsupervised method called Variational Autoencoder (VAE). This approach has two key characteristics: it learns the data distribution to recognize image group characteristics and generates new data based on the reconstructed image to differentiate between two groups: non-porous and porous structures. Our neural network model can help to reduce the time and cost associated with analyzing the mechanical properties of hydrogels in the short term. Moreover, given the ease of data production, our approach may reveal previously unknown mechanical characteristics of hydrogels, opening up new opportunities for tissue engineering and biomaterials development.

Poster Presentation : **ANAL.P-79**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Non-Destructive Depth Profile of Dye-sensitized Photoelectrode with Raman Spectroscopy

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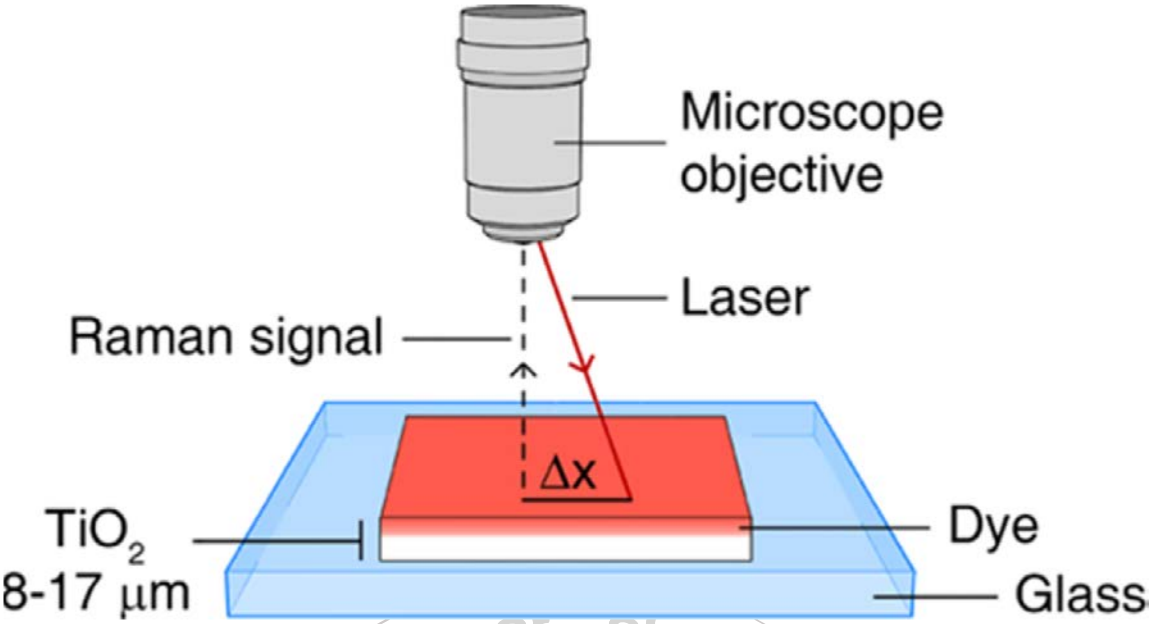
The homogeneous dye distribution within a dye-sensitized photoelectrode is a crucial feature exhibiting superior performance of dye-sensitized photon-to-electron conversion systems such as dye-sensitized solar cells (DSSCs). The chemical environments including dye distribution of the electrode have been investigated by destructive depth profiling means including cross-sectional sampling, which are inappropriate for understanding the internal systems during operations. Hence, a non-destructive evaluation of molecular changes in the devices is necessary for a non-destructive monitoring the dye depth profile. Herein, we present a conceptual demonstration of the dye depth profile within the dye-sensitized anatase TiO_2 layer of photoelectrode of DSSC using a non-destructive/non-invasive Raman spectroscopy, micro-spatially offset Raman spectroscopy (micro-SORS). The depth profile results of TiO_2 layers dye-sensitized with different sensitization conditions demonstrated that micro-SORS can unequivocally discriminate homogeneity of dye sensitization throughout the TiO_2 layers. TOF-SIMS, a representative destructive depth profiling method, exhibited the consistent result with the micro-SORS results. [1] In addition, the internal molecular behaviors in electrolyte of dye-sensitized photo-rechargeable battery (DSPB) during their charging-discharging operation have been monitored using micro-SORS, successfully evaluating changes in relative amount of redox mediator depending on the states of charge of DSPBs. This is the first demonstration of the micro-SORS in the energy conversion systems excluding modification or disassemble of energy devices.


Microscope objective
Laser
Raman signal
Δx
TiO_2
8-17 μm
Dye
Glass

Poster Presentation : **ANAL.P-80**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

CRISPR/Cas-based Nanowire SERS Sensor for Detection of SARS-CoV-2

Ga Eun Jang, Hongki Kim*

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The outbreak of coronavirus disease 2019 (COVID-19) has caused significant social and economic problems worldwide. To effectively treat and manage the spread of the disease, it is important to develop rapid, and accurate diagnostic tools for detecting severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). 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. In the presence of the target RNA, a large amount of final double-stranded DNA products (FPs) is generated through the HIAmp reaction. Then, the FP is specially recognized by Cas12a/crRNA complex and activates the cleavage of Cy5-labeled single-stranded DNA attached to the Au nanowire, resulting in a decrease of SERS intensity. We anticipate that this method may prove effective for the accurate diagnosis of SARS-CoV-2 and expand the application of CRISPR/Cas detecting system.

Poster Presentation : **ANAL.P-81**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

CRISPR/Cas12a-assisted Nanowire sensor for ATP Detection

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The clustered regularly interspaced short palindromic repeats (CRISPR)-Cas12a system has gained considerable attention in molecular diagnostics due to their simplicity, sensitivity, specificity, and broad applicability. The current CRISPR/Cas12a sensing system has been adopted for detecting not only nucleic acids, but also non-nucleic acids, leveraging its collateral cleavage capability. In this study, we report CRISPR/Cas12a based Au nanowire surface- enhanced Raman scattering (SERS) sensor for the detection of adenosine triphosphate (ATP). In the presence of ATP, the locked activators composed of ATP aptamer DNA activator can trigger the release of the DNA activator. Then, the released DNA activator is specially recognized by Cas12a/crRNA complex and activate the cleavage of the Cy5-labeled single-stranded DNA attached to the Au nanowire, resulting in a decrease of SERS intensity. Using this method, it can effectively covert the recognition of ATP into a detectable SERS signal. This study will expand the range of applications for the CRISPR-Cas detection system and provide a practical method for the analysis of non-nucleic acid targets.

Poster Presentation : **ANAL.P-82**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Selectivity of electrochemical reactions by adsorption in confined nanoporous electrodes

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In the field of electrochemistry, increasing selectivity is a very important research topic when using electrodes as catalysts or sensors. Nanoporous electrodes are representative electrode materials for diverse applications, such as catalysts and sensors. Selectivity arising from nanoporous structures has been applied to systems using non-faradaic reactions such ascapacitive deionization, electrochemical supercapacitors, and conductometry. Cases applied to Faradaic reactions have been studied mainly based on reactivity and molecular size. Here, we suggest surface adsorption of reactant molecules as another important factor for selectivity.We observed that a non-adsorption reaction was selectively enhanced more than that of an adsorption reaction at nanoporous electrode due to nanoconfinement effect. This finding may provide insights on the effective utilization of nanoporous electrodes as catalysts or sensors.

Poster Presentation : **ANAL.P-83**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Performance evaluation of thickness-tapered channel in flow field-flow fractionation with field programming

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Flow field-flow fractionation (FlFFF) is an analytical method that can rapidly separate nano to micron-sized particles by sizes without using stationary phase. In FlFFF, the crossflow that is applied perpendicular to the direction of sample migration is closely related with the diffusion of particles and therefore affects both resolution and retention time. Field programming can help separation of large particles by decreasing crossflow rate over time. However, field programming requires an additional high-cost flow controller. In our laboratory, we developed a thickness-tapered channel in which the thickness of the channel decreases along the channel axis, and demonstrated that micron-sized particles can be separated in an increased speed together with the increase of recovery and an expansion of dynamic size range of separation.In this study, we evaluated the performance of the thickness-tapered channel with a conventional channel using field programming with polystyrene latex particles. Larger particles could be separated in the tapered channel, where the inlet thickness (350-100 um) was thicker than the uniform channel (250 um), and particles were separated faster than the uniform thickness channel under the isocratic field conditions. In addition, similar results with field programming were obtained and compared with a thickness-tapered channel.

Poster Presentation : **ANAL.P-84**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A test study on the effect of different decontaminants for A-234

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A-234 is a Novichok A series nerve agent suspected to be employed for Skripal attacks in the United Kingdom and, recently, for Navalny poisoning at the Siberian airport. Since the first confirmed Novichok attack in 2018, its compounds are being increasingly investigated; however, experimental data on their effective decontamination remains scarce. Therefore, herein, we attempted to investigate the decontamination of A-234 to understand its potential risk to the environment through different analytical methods, including liquid 31P NMR, GC-MS, and LC-MS. Our results showed that the agent did not break up easily in water or with dichloroisocyanuric acid sodium salt, sodium persulfate, and chlroine-based water-soluble decontaminants but was efficiently decontaminated by Oxone monopersulfate, calcium hypochlorite, KOH, NaOH, and HCl within 30 min. Our findings can contribute to the knowledge on how A-234 can be eliminated to reduce its enviornmental impact.

Poster Presentation : **ANAL.P-85**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation of lipidomic perturbations in feces and saliva from lung cancer patients

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Lung cancer is a fatal disease with the highest incidence and mortality. Most lung cancer patients are found in situations that radical surgery is difficult, because of the lack of early diagnosis methods and the difficulty in obtaining invasive samples. Therefore, it is necessary to develop new biomarkers from non-invasive and easily available samples.Lipid profiling for diagnostic purposes has become one of the promising area in relation to metabolomic approach. Nevertheless, studies of fecal and salivary lipids as potential biomarker candidates have not been thoroughly investigated. Feces and saliva from patients with lung cancer may have significant alterations in lipid profiles. Therefore, lipidomic analysis of fecal and saliva samples from patients with lung cancer is necessary.In this study, lipid profiles of fecal and saliva samples from lung cancer patients (LC, n = 26) together with controls (C, n = 22) were analyzed by nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Total 206 lipids were identified and 166 lipids were quantified in feces, while total 634 lipids were identified and 304 lipids were quantified in saliva. As a result, in fecal samples, PC, PG, Cer, and CE lipids increased in LC group. On the other hand, PI and DG lipids showed decrease in the LC group. While most lipids in saliva were decreased in the LC group, DG and TG lipids were increased in the LC group. Among the lipids showing significant changes, 6 lipids in feces and 36 lipids in saliva were finally determined as biomarker candidates.

Poster Presentation : **ANAL.P-86**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development and Characterization of Spiropyran-based Photo-switchable Stationary Phase for Microfabricated Gas Chromatography.

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[1]*Center for Sustainable Environment Research, Korea Institute of Science and Technology, Korea*

In this work, we developed and characterized a novel photo-switchable stationary phase for micro gas chromatography (μGC) to separate gas samples having various polarities. The UV curable polymer was used as the stationary phase composed by a copolymer of acrylic acid (AA), methyl methacrylate (MMA), 2-{3’,3-dimethyl-6-nitro-3’H-spiro[chromene-2,2’-indole]-1-yl}ethanol (SPOH), and Darocur using a dynamic method. For uniform coating of the stationary phase, the dynamic method was applied. This method supplemented the disadvantage of the static method, which is difficult to control the coating thickness due to multiple procedures. For photo-switching, a UV transparent copolymer of MMA and AA was chosen as the polymer backbone. Spiropyran derivatives (SPOH) are relatively nonpolar and can be reversibly switched to a polar, zwitterionic merocyanine isomer. This reversible transformation can be shown under UV-visible light. As 250 – 380 nm irradiation was applied, the C-O bonds of SPOH were broken and form into its color-emitting MC form. Once the irradiation has stopped, the MC started to colorless and revert to its original form, the SPOH. The contact angle measurements exhibited a reversible hydrophobic-hydrophilic properties from 80° to 55° $\Delta\theta$ upon alternating UV and visible irradiations. Photoreversibility was observed after 10 cycles of UV-Vis exposure without specific loss in the optical performance. The thickness of the stationary phase and separation efficiency were investigated by Field Emission Scanning Electron Microscopy and Gas chromatography with flame-ionization detection. As the polarity of the column changed, the separation results showed distinct changes in retention behaviors of the mixture of benzene, toluene, ethylbenzene, alcohols, and ketones.

Poster Presentation : **ANAL.P-87**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

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

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Human skin functions as a primary physical barrier against the external environment. The main constituents of stratum corneum, the outermost layer of epidermis, are lipids such as ceramides and glycerolipids. Tape stripping is one of the most efficient skin sampling method. 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 was focused to optimize skin sampling method in terms of sampling location and the number of tape strips in case of repeated stripping. Skin samples from ten sequential tape strips from the same spot and those from five sequential tape strips from 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. As the skin samples were taken from a same location repeatedly, the amount of identified lipid species had a tendency to decrease along with the slight variations in lipid composition, and it was largely decreased 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. More than 100 lipid species were in addition identified from pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strip for sample pooling, variation in lipid composition and amounts among the adjacent spots was evaluated in advance. 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. Sample pooling was adopted to establish the most representative tape stripping method that can represent skin lipid composition and avoid loss of any other quantifiable lipids.

Poster Presentation : **ANAL.P-88**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Lipidomic analysis of serum exosomes from patients with cholangiocarcinoma by nUHPLC-ESI-MS/MS and FlFFF-ESI-MS/MS

Hyeju Yu, Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Cholangiocarcinoma is divided into intrahepatic cholangiocarcinoma and extrahepatic cholangiocarcinoma according to the site of origin. It is necessary to differentiate and diagnose the type of cholangiocarcinoma because the treatment methods are different. However, early detection of cholangiocarcinoma is difficult, and the mortality rate is high within 5 years after diagnosis. Therefore, it is necessary to specify a biomarker candidate group capable of distinguishing and diagnosing cholangiocarcinoma.Exosomes are one of the extracellular vesicles (EVs) that are externally released from cells. Exosome contains lipids, proteins, and nucleic acids of the parent cell and closely related to intercellular communication. Therefore, exosomal lipids can serve as biomarkers of disease. Ultracentrifuge, size exclusion chromatography, and size-based filtration method are used for exosome isolation, but each method has its own strengths and weaknesses. Asymmetrical flow field-flow fractionation (AF4) can be utilized as an alternative method for separating/isolating exosomes according to their size. Since AF4 separates particles and macromolecules only with the interaction of flow streams without utilizing packing materials as in chromatography, a possible sample interaction with stationary phase can be removed when biological particles are considered for separation. In this study, the minimum volume of serum capable of exosome lipid analysis was optimized due to the limited volume of patients' serum sample. Exosome lipid analysis of patients serum was optimized to 0.5 mL of serum. For the top-down lipid analysis of exosomes depending on sizes, a miniaturized AF4 channel was constructed in laboratory in order to directly hyphenate it with mass spectrometry (MS) via electrospray ionization (ESI). First of all, a flow optimization was accomplished to separate particles in the size range of the exosomes (30-100 nm) within 10 minutes by varying channel thickness and flow rate in the miniaturized AF4 channel. Secondly, the miniatured AF4 channel was hyphenated with ESI-MS/MS, and the best ionization conditions are being optimized by altering the flow rate of the modifier and sheath gas and realigning the position of the HESI -II probe.


사단법인 대한화학회
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Poster Presentation : **ANAL.P-89**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Lipidomic analysis of mice brain and spleen with SARS-CoV-2

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SARS-CoV-2 (severe acute respiratory syndrome coronavirus) has caused pandemic in the past three years. While most people recover from the disease except few severe illness, there are a number of people suffered from loss of taste or smell, fatigue, headache, muscle aches, and diarrhea besides respiratory symptoms. Moreover, although there are many evidences that viral infection occurs in various tissue other than lungs, lipidomic analysis has rarely been conducted so far except for blood, plasma, or serum.Lipids are not only used as energy sources and cellular components, but are also involved in signal transduction and permeability of cell membranes. Due to these various role of lipids, viral infection is expected to induce significant alternations in lipids in metabolic pathway.For investigate lipid perturbation by the SARS-CoV-2, qualitative and quantitative analysis have been performed in the brain and spleen tissues of transgenic mice expressing the human angiotensin converting enzyme 2 driven by the k18 promoter. In this study, brain and spleen samples were obtained from mice groups at six different time points (1, 2, 5, 7, 10, and 14DPI (day post infection) with two different plague forming unit (PFU) along with control and their lipid profiles were examined using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS).As a result of qualitative analysis, a total of 593 and 926 lipids were identified from the brain and spleen samples, respectively. Compared to the brain acyl chains of TG and phospholipid were more diverse in spleen. From targeted quantification, LPC, known to be associated with inflammation showed a decrease during infected periods, but PC showed an increase with the increase of PFU. Quantitative analysis of other lipid classes at the molecular level is still on going and their results will be introduced.

Poster Presentation : **ANAL.P-90**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Evaporation characteristics of Novichok according to the alteration of volume and wind velocity on the diverse materials

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Chem-Bio Technology Center, Advanced Defense Science & Technology Research Institute, Agency for Defense Development, Korea

Historically, chemical warfare agents (CWAs) had been developed and used by some countries to cause severe threat during the war. CWAs pose widespread and constant damage to terrorized region because deadly vapor is continuously produced as long as they remain on the ground. Therefore, it is necessary to study evaporation of CWAs. Especially, research on Novichok, the newly registered CWA to Chemical Weapon Convention (CWC) by Organisation for the Prohibition of Chemical Weapons (OPCW) is highly needed since several terrorist attacks using Novichok have occurred recently (e.g. Skripal poisoning and Navalny poisoning). In this report, we analyzed the evaporation characteristics of Novichok (A-232) on the various materials such as concrete, sand, and glass according to the alteration of wind velocity. We generated the air boundary layer stably on the material with A-232 on it by using wind tunnel, controlling the temperature and humidity of the air flow with a flow generator. In addition, evaporation of A-232 without wind flow was either studied. For the windless condition, micro-chamber thermal extractor (m-CTE) was used to maintain constant temperature excluding air flow. The exhaust from wind tunnel and m-CTE was caught by adsorption tubes and analyzed by thermal desorption-gas chromatography. Novichok vapor was increased as temperature rose on the diverse materials in both windy and windless conditions and the wind flow had a significant impact on the vapor generation.

Poster Presentation : **ANAL.P-91**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Chiropticality of Magnetoplasmonic nanoparticle-doped titania hydrogels and aerogels

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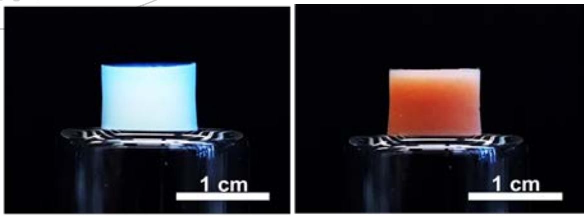
Department of Chemistry, Chungnam National University, Korea

Aerogel is a type of solid-phase material formed by the coordinated networking of organic or inorganic matters, which result in an open and highly porous 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 weigh only 0.13 grams per cubic centimeter and possess UV-visible broad absorption, which were modulated by the amount of doped MagPlas NWs. The combination between highly UV-absorbing TiO_2 anatase and magnetoplasmonic core-shell nanowires allows utilization of both UV- and visible spectrum range of light, which potentially enhances the light-harvesting efficiency and photocatalysis applications. Furthermore, the magnetic susceptibility of the gold-magnetite nanowires also allows unique arrangements in TiO_2 hydrogels, which opens up possibilities for self-assembly into unique linear and helical superstructures.



Poster Presentation : **ANAL.P-92**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Harnessing the surface structure to enable high-performance olivine cathode mateirals for Lithium-ion batteries

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The high-performance cathode materials is often the critical limiting factor in improving lithium-ion batteries (LIBs). Among all the reported cathode materials for LIBs, olivine-type cathodes have received particular attention in the past decade due to their successful commercialization in diversified electric vehicle (EVs). Currently, there is a focus on developing a high-voltage olivine battery to increase energy density, due to its many advantages over conventional batteries. While studies mainly focus on the macroscopic and bulk crystal structure of the olivine materials, our work suggests that the electrochemical performances of the interfacial structures of cathode materials should also be regulated, as they are the confined regions where charge transfer takes place. In this study, a hybrid coating layer containing carbon (C) and $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) has been applied to high-voltage $LiFe_{0.4}Mn_{0.6}PO_4$ and $LiFe_{0.4}Mn_{0.3}Co_{0.3}PO_4$ cathodes. Our investigation reveals that the coated layer simultaneously supplies electrons and enhances Li-ion transportation, greatly improving electrochemical performances, including specific capacity, rate capability, and cycling stability.

Poster Presentation : **ANAL.P-93**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synergistic strategy of europium-doped magnetoplasmonic nanoparticles for aqueous copper(II) sensing

My-Chi Thi Nguyen, Huu-Quang Nguyen, Jaebeom Lee[*]

Department of Chemistry, Chungnam National University, Korea

Luminescent lanthanide compounds are of interest in imaging, sensing, and catalysis applications owing to their sharp emission and high resistance to photobleaching. Here, europium ion was doped into hybrid magnetoplasmonic nanoparticles which inherit high photoluminescence efficiency and strong magnetic characteristic. The incorporation of fluorescent lanthanide and Ag@Fe_3O_4 nanoparticles has effectively boosted photoluminescence, attributed to the existence of core-shell structure and plasmon silver core. The as-synthesized NPs exhibit as a sensing probe in environmental technology because photoluminescence is selectively and sensitively quenched when encountering copper (II). This heavy metal ion can be possibly removed by intrinsic magnetic NPs. These results suggest that the complex of Eu-doped magnetoplasmonic NPs can be assigned to be an effective sensing material for aqueous copper(II).

Poster Presentation : **ANAL.P-94**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation of Two-dimensional Multilayered Iron Selenide Nanosheets using Electrochemical Methods

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The iron selenide is one of the transition metal chalcogenide compounds, also it is well-known as the superconductive material at ultralow temperature(8K). Furthermore, the L-cysteine ligands coupled FeSe quantum dots had been reported for their unique multi-colored excitation dependent emission property, and the FeSe quantum dots have been proved successfully their biomedical imaging application to target breast tumor cell. Otherwise, even though the FeSe has been reported its multilayered structures, but the trials to exfoliate it into single or a few layers, and electrochemical experiment to investigate FeSe characters and application is rarely reported. Therefore, we investigated electrochemical properties to compare two different size of FeSe nanomaterials(3.6 nm, 500 nm) using glassy carbon electrodes and FTO(Fluorine-doped Tin Oxide) glasses as working electrodes. The main goal is finding size-dependant electrochemical characteristics by cyclic voltammetry and EIS (Electrochemical Impedance Spectroscopy) plots, and looking for opportunity to apply FeSe into another conventional electrochemistry fields.

Poster Presentation : **ANAL.P-95**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

SERS detection of shikonin dye by metal-coordinated tethering and NPoM

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We developed a spectroscopic detection method of dye molecules by combining surface-enhanced Raman spectroscopy (SERS) and a metal-coordinated tethering method. In order to mimic the surface of cellulose fiber, a gold nanofilm (AuNF) surface was modified with hydroxyl groups, and then treated following a tethering process to form a metal ion-mediated dye ligand complex (Al^{3+}-shikonin dye complex) on the AuNF. Then, the colloidal gold nanoparticles (AuNPs) were dropped and dried to form SERS hot-spots, where shikonin locates in the interstitial gap between AuNP and AuNF. The SERS enhancement factor (EF) of AuNP-on-AuNF was calculated to be 4.4×10^7 via SERS measurement of 4-mercaptobenzoic acid (4-MBA). The SERS heatmap of shikonin from the ‘dyed AuNP-on-AuNF’ substrate showed that shikonin was uniformly tethered on AuNF surface in the same way as the dyeing of dye molecules on cellulose fibers. 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. This method can apply to various natural dyes owing to the versatility of the dyeing method with a metal ion. Moreover, SERS libraries obtained using this method can directly compare with dyes tethered on fibers.

Poster Presentation : **ANAL.P-96**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Yolk-shell structured carbon coated Fe3BO5 as an anode material for high C-rate lithium ion battery applications

Rajeev Kumar, Jeongin Kim[1], Youngil Lee[1,*]

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Yolk-shell structured, carbon-coated vonsenite (Fe3BO5) were synthesized by the solid-state method and utilized as conversion-type anode materials. The core consists of vonsenite nanoparticles, while the shell is composed of a defective (partially graphitized) carbon layer. A higher synthesis temperature leads to the formation of larger amounts of metallic impurities as a result of the carbothermal reduction. The electrochemical characteristics of the sample synthesized at an optimum temperature of 600 °C were better than those of the sample synthesized at higher temperatures and without the carbon coating. This can be attributed to the smaller-sized crystallites having the least amount of metallic impurities and a better-formed solid electrolyte interphase (SEI). This optimized sample demonstrated an outstanding reversible specific discharge capacity of 976 mAh g-1 at a current density of 0.05 A g-1. Long cyclability test at an ultra high C-rate of 5 A g-1 outlined the critical role of an effective SEI and carbon coating. The origin of the capacity values higher that the theoretical value of 726.3 mAh g-1 is also investigated. Remarkably, this sample demonstrated electrochemical activity even upto a C-rate of 20 A g-1, thus validating the usefulness of this material as a safe and stable anode for fast charging-discharging Li-ion battery applications.

Poster Presentation : **ANAL.P-97**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ultra-Sensitive Fluorescence Sandwich Immunoassay for Small Molecule Detection

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To overcome the sensitivity limit in immunoassays for small molecules (haptens), we established a fluorescence sandwich immunoassay that can detect hapten molecules in the zeptomole range. Our platform is based on the biotin-avidin system-based dual epitope sandwich type noncompetitive immunoassay. Gold nanoplate-based biotin antibody and streptavidin-Alexa fluor488 (SA-Flu) were used instead of streptavidin-HRP (SA-HRP) reacting with biotin-tracer included in a commercial microplate-based competitive ELISA kit. Histamine (HIS, 111.148 Da), which plays a central role in the pathogenesis of several allergic diseases, was chosen as the target hapten model. We demonstrated through total internal reflection-based optical microscopy that nanoprobe (SA-Flu) fluorescence intensity increased with increasing target concentration (HIS) after sandwich immunoreaction on gold nanoplates. This method showed 5.4 x 10^{10} times better sensitivity than the existing competitive ELSIA method, which is a tune-off format. Therefore, novel small molecule fluorescence sandwich immunoassay (smFSIA) on gold nanoplate provides an extremely low detection limit (~zM), a very wide measurable range, and practical specificity for quantitative analysis of small molecule.

Poster Presentation : **ANAL.P-98**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Timeseries spectroscopic study of Optical Redox Ratio

Jin Il Jang

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Autofluorescence is a non-invasive analysis method which is used to diagnosing for in vivo and ex vivo tissues. Normally, Autofluorescence appears at a wavelength of 400 nm to 700nm and includes various biometric information. Among them Nicotinamide dinucleotide (NADH) and Flavin adenine dinucleotide (FAD) are co-enzymes used in metabolism and respirations, which are strongly associated with pathological symptoms, Optical Redox Ratio (ORR) is a ratio of fluorescence intensity of NADH and FAD. ORR is used as indicators for diagnosing lesion and cancer tissue. However, ORR has a various result of research on tissues and few reports have been reported on evaluating the variation of ORR value over time. In this study, For the evaluation of ORR indicators, a mixed solution of NADH and FAD was prepared at a concentration similar to that of biological conditions, and time series analysis of absorption and fluorescence was measured. The ORR value was obtained by deconvoluted each spectrum of NADH and FAD in the spectrum of the mixed solution. It was observed that the fluorescence spectral region of NADH decreased and FAD was uniform over time. This is due to the oxidation-reduction coupled reaction of NADH and FAD. In addition, fluorescence intensity of both NADH and FAD decreased when measuring fluorescence, which is an effect by the inner filter effect, and these effects tend to increase ORR values over time. Based on the spectroscopic study, we concluded that ORR values need to be calibrated before using them as a spectroscopic diagnostic marker.

Poster Presentation : **ANAL.P-99**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Inkjet printing of multifunction electrodes on a paper used as a novel of affordable and rapid PCR device

Sarath Kin, Kwanwoo Shin*, Semin Chun, Eunjin Huh, Ignasia Handipta Mahardika, Oh-Sun Kwon

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Paper-based devices are preferred in point-of-care testing (POCT), particularly in biomedical sensors, to improve ASSURED guidelines: affordable, sensitive, specific, rapid/ robust, equipment-free, and deliverable to end-user. Conductive patterns deposited on a paper substrate via simple inkjet printing and the optimization of the voltage, current, and resistance applied to the patterns, enable paper-based electrodes to manipulate, heat, and sense a low volume sample drop for either sample pre-treatment or detection. The potentials of these multifunctional paper-based electrodes have also been shown to be applicable in polymerase chain reaction (PCR) for DNA amplification. Recently, miniature size on-chip PCR devices have been fabricated. However, glass, monocrystalline silicon, and printed circuit boards (PCBs) are used as substrates, making the manufacturing process complicated, expensive, and harmful to the environment. Herein, we introduce the novelty of a simple, eco-friendly, and affordable paper-based PCR device using inkjet-printed patterned versatile electrodes on photopaper. Our paper-based PCR device was assembled by integrating a paper-based electrowetting-on-dielectric (EWOD), microheater, and temperature sensor to transport, heat, and sense the sample droplets, respectively. The entire paper-based chip was made by simply printing the silver nanoparticles (AgNPs) conductive ink (combined with PEDOT:PSS polymer ink for temperature sensor) on Kodak Photopaper using different design patterns (to make different functional electrodes). Plus, additional treatments including polysulfone (PSU) dielectric and Teflon hydrophobic layers were deposited onto the paper-based chip to adjust the contact angle of the droplets and sustain high electric fields for repeated cycling. Our paper-based EWOD shown the ability to mix and transport droplets back and forth for more than 40 cycles, while the microheater could generate temperature of more than 100 celcius degree (5 × 10 mm, R = 75 Ω), and the seebeck coefficient of a temperature sensor between interfacial junction of PEDOT:PSS and AgNPs was 18.873 μV/K. The combination of these components into a single paper-based PCR device will become a new technology, which allow DNA amplification to be more convenient and less expensive than traditional methods. Keywords: Point-of-care testing, PCR amplification, Inkjet printing, Paper-based multifunction electrodes, EWOD, micro heater, thermocouple temperature sensor.

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Poster Presentation : **ANAL.P-100**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Lipidomic profiling on effects of intermittent diet in high fat diet-induced NASH mice using LC-MS

Yeajin Ju, Geum-Sook Hwang*

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Altered lipid composition is one of the major reasons for nonalcoholic fatty liver disease (NAFLD). To date, no specific drug has been established, so intermittent fasting (IF) could be a new treatment strategy. Therefore, this study analyzes the therapeutic effect and underlying mechanism of intermittent fasting in NAFLD. In this study, C57BL/6J mice (male) were fed a normal diet (ND) and high-fat diet (HFD) and subjected to an alternated-day diet after 12 weeks for 35 weeks. Then, we performed global lipid profiling with liver from mice to estimate metabolic alteration using ultra-performance liquid chromatography/quadrupole time of fight mass spectroscopy (UPLC/Q TOF MS). Principal component analysis (PCA) score plots showed a separation between four groups in negative ion mode, however, there was only a difference in dietary effects in positive ion mode. We identified a total of 223 lipids. Most phosphatidylcholine was decreased in high-fat diet mice and showed a recovery pattern with intermittent fasting mice on high-fat diet mice. This study demonstrated that lipidomic profiling with LC-MS is a useful method to investigate the effects of intermittent fasting in obese mice.

Poster Presentation : **ANAL.P-101**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Fabrication and Characterization of Fiber-Optic SERS Probes Conjugated with Gold Nanoshells

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SERS is a non-destructive and ultrasensitive method for detecting molecules, and it is based on localized surface plasmon resonance (LSPR) caused by metal nanoparticles attached to a substrate. The use of optical fibers as a substrate allows for more flexibility in detection, such as remote sensing. SERS measurements using optical fibers require the addition of plasmonic nanostructures to the end of the fiber. But the conventional method for creating metal structures in the end-facet of a fiber substrate involves complex lithography processes.In this study, we fabricated a fiber-optic SERS (FO-SERS) probe with relatively easy wet chemistry conditions. To achieve this, gold nanoshells which are composed of a silica core and surrounding gold nanoparticles were chemically conjugated to the end of the fiber. The resulting probe was characterized by scanning electron microscopy (SEM), confirming that each nanoshell was conjugated at the fiber end-facet by monolayer. The signal of FO-SERS was detected in the optrode configuration. This method is expected to be simple and inexpensive. Overall, this study contributes to the development of SERS-based fiber-optic probes for ultrasensitive molecular detection.

Poster Presentation : **ANAL.P-102**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Flow-Controlled Lateral Flow Assays for a High Sensitivity Detection of Biomolecules

Ignasia Handipta Mahardika, Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea

The Lateral Flow Assays (LFAs) technology has seen an unprecedented growth due to the crisis and relevant countermeasures adopted after the global spread of the COVID-19 crisis virus. LFAs have several advantages, such as ease of use and widespread accessibility while also being environmentally friendly and employable by countries with limited medical infrastructure. Although being a promising technology, LFAs also comes with several complications. The isotropic wicking properties of the paper substrate which results in variations of the flow rate, one of the key parameters when it comes to the chemical reactions of and between biomolecules. To this aim, and improvement in the design capabilities of the flow rate shall allow for a higher degree of control of the reaction time of biomolecules, resulting in an improvement of the signal intensity of the LFAs.To address this issue, in this research, hydrogel, as the most biocompatible material, was introduce in the LFAs system. Accordingly, various concentrations of poly(ethylene glycol) diacrylate (PEGDA) hydrogel were coated on a nitrocellulose membrane providing the control of the solution flow given by the designed porosity. To demonstrate the reliability of the proposed solution, the hydrogel-coated LFAs was employed for the lab-scale manufacturing of a pregnancy detection test. In comparison to hydrogel-free strips, volume concentrations of hydrogel between 6% and 9% already resulted in a T/C intensity improvement between 10% and 35%. In addition, when the concentration is increased to 12%, the detectability reaches its maximum with an improvement close to 40%. It is also interesting to highlight that, for hydrogel concentration higher than 12% the T/C intensity decreases as a consequence of the excessive drag caused by the hydrogel, which has a negative effect on the flow rate.Keywords: lateral flow assays, hydrogel, PEGDA, flow control

Poster Presentation : **ANAL.P-103**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nanoplasmonic assay platforms for reproducible SERS detection of Alzheimer’s disease biomarker

Hajun Dang, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

With the recent developments in high-sensitivity optical detection technologies, many studies have been conducted to accurately detect biomarkers with low concentrations of 1.0 pM or less and apply them to in vitro diagnostics. The tubulin-associated unit (tau-381) protein, a biomarker of Alzheimer's disease, is a representative example, and its cut-off value reported in clinical practice is 5.5 fM. Therefore, a robust sensing technology that detect such low concentrations of biomarkers is needed. In this study, tau-381 was detected with high sensitivity and reproducibility by a plasmonic Au nanopopcorn substrate fabricated via thermal evaporation. Here, aptamer DNAs labeled with Raman reporters on the terminal were used as the receptors. The plasmonic nanopopcorn substrate used in this study is composed of uniform gold nanoparticles (AuNPs) of an average size 64 nm. The reproducibility was significantly improved through more uniform nanogaps than those formed by aggregation of AuNPs in solution. An assay was conducted by first reacting tau-381 with the corresponding aptamers, and the remaining aptamer DNAs were then reacted with capture DNAs immobilized on the surface of the Au substrate. The assay results for tau-381 showed a detection limit value of 2.2 fM, below the cut-off value (5.5 fM).

Poster Presentation : **ANAL.P-104**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Laser-induced breakdown spectroscopy (LIBS) signal enhancement by aligning analytes along the pre-defined laser-ablation pathway

Hanbeom Choi, Yonghoon Lee*, Sang-Ho Nam*

Department of Chemistry, Mokpo National University, Korea

In this work, we devised a new solid substrate on which salt crystals are well aligned along the pre-defined laser-ablation pathway. Parallel 1-cm long trench lines were carved in 1 cm X 1 cm area on the silicon wafer by laser patterning. Then, along the four sides of the area, scotch tapes were attached enclosing the laser-patterned area. Salt samples were prepared in forms of aqueous solutions, and a drop of each solution was dropped on the area. The droplet formed a thin square film well fitting to the square area. After water was evaporated, residual salt crystals were observed to lie along the laser-produced trenches. This can be ideal sample for laser-ablation-based elemental analysis. For LIBS analysis, nanosecond laser pulses were launched along the pre-produced trench lines on which salt crystals had been located. This increased Mg, Ca, and K emission line intensities and thus provided remarkably improved sensitivity for the analysis of these elements in edible salt products.

Poster Presentation : **ANAL.P-105**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Studying Semiconductor Nanoparticles by MALDI-MS with Various Matrices

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Mass spectrometry, particularly matrix-assisted laser desorption ionization mass spectrometry (MALDI-MS), is a widely used technique in nanoparticle research, including studies of quantum dots (QDs). Improving the low ionization efficiency of QDs in MALDI-MS is a significant challenge in QD research In MALDI-MS, the ionization efficiency is highly dependent on the choice of matrix, which acts as a support for the ionization process. In this study, we investigate the ionization efficiency of QDs with several matrices in MALDI-MS. Two ionization mechanisms for QDs in MALDI-MS were proposed: 1) after the matrix absorbs the 337 nm laser to become cation radicals, the QDs are ionized, and 2) after the QDs absorb the 377 nm laser, the matrix takes electrons from the excited QDs. According to the suggested mechanism, the better the electron acceptor matrix, the higher the possibility of higher ionization efficiency of QDs. Remarkably, porphyrin-based matrices showed superior performance compared to conventional matrices in terms of mass spectrum intensity for all types of QDs, demonstrating enhanced electron transfer. Porphyrin-based matrices act as effective electron acceptors and can efficiently remove electrons from excited QDs. Furthermore, we can observe that chorine-passivated QDs have lower ionization efficiency than non-chlorine-passivated QDs. Even in the case of chlorine-passivated QDs with poor ionization efficiency, we expect that analysis through MALDI-MS will work well if the appropriate matrix is used. In conclusion, this study provides insight into the effect of matrix properties on ionization in MALDI-MS, and the use of porphyrin-based matrices has the potential to improve QDs analysis greatly.

Poster Presentation : **ANAL.P-106**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a High-Performance Photoionization Detector Using Spiral Micro-electrodes.

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Volatile organic compounds (VOCs) are the organic compounds which can easily volatilize into the air due to their low boiling points. VOCs have potential adverse effects on the human health such as disorders in the nervous system and respiratory disease upon exposure. Therefore, it is necessary to monitor VOCs in real-time with high sensitivity. Several analytical techniques have been applied to detect VOCs. Among them, gas chromatography (GC) is the standard analytical method of separating and detecting each VOC. Photoionization detector (PID) is one of the detectors have been typically used in GC which utilize high energy (10.6 eV) from ultraviolet light(UV) to ionize VOC with high sensitivity and selectivity. However, it is still difficult to use in the field due to its large size and low sensitivity, thus needs to be miniaturized. In this study, we developed PID using micro-electrodes to improve the sensitivity. The micro-electrodes were fabricated on the silicon wafer which was designed in the form of spiral to increase the area where the sample was photoionized. In addition, its shape was optimized by adjusting the distance between the electrodes to 200, 250, and 300 μm. The sensing performance was improved by adding an oxide layer and a Pt electrode layer to the silicon wafer. The PID was evaluated with the mixtures of benzene, toluene, ethylbenzene, and xylene and compared to the existing sensing performance. To minimize the electrode photoelectric effect on Si, a Pt electrode layer was added to stabilize the baseline of the signal. Compared to the existing PID that requires a long time to be performed, the stabilization time was significantly reduced by removing residual electrons.

Poster Presentation : **ANAL.P-107**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A simple strategy to improve SERS detection sensitivity in a small volume well-plate

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Surface-enhanced Raman scattering (SERS)-based sandwich immunoassay has been used to analyze target antigens using antigen-antibody interaction quantitatively. Capture antibodies are immobilized on the two-dimensional surface of a 96 well-plate, and then target antigens and SERS nanotag-labeled antibodies are sequentially combined to form sandwich immunocomplexes. One could perform the quantitative analysis of a target antigen by monitoring the characteristic Raman peak intensity of the SERS nanotag after creating sandwich immunocomplexes. However, immunocomplexes formed on a two-dimensional surface have a limitation in loading density due to a limited surface-to-volume ratio, resulting in poor sensitivity. In addition, when using a 96-well plate, a large sample volume is required for one well, and there is a limit to high throughput assay. To resolve these problems, we developed a highly sensitive SERS-based assay platform using SiO2 microparticles and a 1536-well plate. It was possible to improve the detection sensitivity of a target by increasing the surface-to-volume ratio with three-dimensional SiO2 microparticles. When performing the SARS-CoV-2 assay using the proposed platform, the detection limit could be improved more than ten times compared to the assay result using a 96-well plate-based absorbance enzyme-linked immunosorbent assay (ELISA).

A simple strategy to improve SERS detection sensitivity in a small volume well-plate

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Surface-enhanced Raman scattering (SERS)-based sandwich immunoassay has been used to analyze target antigens using antigen-antibody interaction quantitatively. Capture antibodies are immobilized on the two-dimensional surface of a 96 well-plate, and then target antigens and SERS nanotag-labeled antibodies are sequentially combined to form sandwich immunocomplexes. One could perform the quantitative analysis of a target antigen by monitoring the characteristic Raman peak intensity of the SERS nanotag after creating sandwich immunocomplexes. However, immunocomplexes formed on a two-dimensional surface have a limitation in loading density due to a limited surface-to-volume ratio, resulting in poor sensitivity. In addition, when using a 96-well plate, a large sample volume is required for one well, and there is a limit to high throughput assay. To resolve these problems, we developed a highly sensitive SERS-based assay platform using SiO_2 microparticles and a 1536-well plate. It was possible to improve the detection sensitivity of a target by increasing the surface-to-volume ratio with three-dimensional SiO_2 microparticles. When performing the SARS-CoV-2 assay using the proposed platform, the detection limit could be improved more than ten times compared to the assay result using a 96-well plate-based absorbance enzyme-linked immunosorbent assay (ELISA).

Poster Presentation : **ANAL.P-108**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a SERS-based assay platform using CRISPR-Cas12a for sensitive molecular diagnostics of COVID-19

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[1]*Chung-Ang University, Korea*

Since November 2019, the COVID-19 pandemic is still ongoing globally. The current gold standard for detecting the SARS-CoV-2 target gene is RT-PCR. However, since this technology cannot detect the extracted target gene as it is due to the sensitivity limit of the fluorescence detection method, the amplification process of the target gene using the thermocycling process is needed. To implement amplification-free detection of the SARS-CoV-2 gene, we developed a susceptible SERS detection technology based on CRSIPR-Cas12a. First, SARS-CoV-2 RNA was amplified to double-strand DNA by RT-LAMP and then used as an activator for the trans-cleavage of the Cas12a protein. Subsequently, SARS-CoV-2 was quantified by monitoring the change in Raman intensity when the single-strand DNA immobilized on the Au nanopopcorn substrate was cut by the CRISPR/Cas12a system. This presentation will introduce a CRISPR/Cas12a-based SERS assay platform that can quantify SARS-CoV-2 with high sensitivity.

Poster Presentation : **ANAL.P-109**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Lipidomic analysis in aorta tissue from ApoE knockout mice model of diabetes induced atherosclerosis using LC/MS

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Atherosclerosis is the leading cause of most cardiovascular diseases, and diabetes is known to accelerate the progression of atherosclerosis. However, the mechanism of diabetes-accelerated atherosclerosis is still not fully understood. In the present study, we investigated the alteration in lipid metabolism related to diabetes in atherosclerosis using liquid chromatography tandem mass spectrometry (LC/MSMS).5-week-old ApoE knockout mice were designed three groups: normal diet (ND) group fed a normal diet, high fat diet (HFD) group fed a high fat diet, and streptozotocin (STZ) group fed a high fat diet and injected with STZ. Aorta tissues were obtained by sacrificing 10-week-old and 12-week-old mice.Partial least squares-discriminant analysis (PLS-DA) score plots showed a clear separation between HFD and STZ groups compared to the ND group in positive and negative modes, respectively. A total of 228 lipid metabolites were identified in aorta tissues. Especially, phosphatidylglycerols (PGs) and triacylglycerols (TAGs) were significantly changed in the HFD group compared to the STZ group. PGs were observed to promote atherosclerosis in diabetes by a specific chain at 12 weeks and TAGs were confirmed to have a unique pattern according to chain length and presence of diabetes.Our finding suggested that PGs might accelerate atherosclerosis in diabetes and demonstrated that lipidomic profiling using LC/MSMS is useful for understanding aorta lipid metabolism in diabetes induced atherosclerosis mice.

Poster Presentation : **ANAL.P-110**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and electrochemical studies of $Zn_3(BO_3)_2$ material as an anode material for Li-ion batteries

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[1]*Chemical Industry Research Institute, University of Ulsan, Korea*

Commercial anode material such as graphite and lithium titanate have good cyclability but relatively lower specific capacity. In contrast, Si-anodes have a very high specific capacity but suffer from large volume change during cycling. Thus, development of safe anode materials with high performance in terms of both cyclability and specific capacity, is crucial for the successful application of Li-ion batteries. In this study, conversion-type anode materials, i.e., transition metal borates, as promising candidates for Li-on storage are evaluated. In particular, $Zn_3(BO_3)_2$ has been synthesized by conventional solid-state reaction method and used as anode material for Li-ion batteries. $Zn_3(BO_3)_2$ is a good material as an anode with a theoretical capacity of 512.5mAh/g. The electrochemical tests using the 2032 type coin cell of the material for Li-ion battery were evaluated after the prepared sample was characterized by X-ray diffraction (XRD) and thermal weight analysis (TGA). The good results of cyclic voltammograms, long cycling, and rate performance validate its usefulness as a stable and high capacity anode material.

Poster Presentation : **ANAL.P-111**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Electrochemical Reactions Affected by EDL Overlapping in Nanoporous Electrodes

Jinju Kim, Hyun Ju Yang, Je Hyun Bae[*]

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

When a potential is applied to an electrode in a solution containing an electrolyte, an electric double layer (EDL) is formed as ions having a charge opposite to that of the electrode are gathered around the electrode. The EDL is important because electrochemical reactions take place in the layer. Unlike flat electrodes, the EDL overlaps in nanoporous electrodes. EDL overlapping in nanoporous electrodes has been mainly studied in the charging behavior of ions, and not much in the Faraday reaction. In this study, we explore that electrochemical reaction can be controlled by EDL overlapping in nanoporous electrodes by chronoamperometry. We confirmed that the electrochemical reaction is controlled by electrolyte concentration, measuring time, overpotential, and ionic size because of the EDL overlapping. These findings may provide insight into utilization of nanoporous electrodes as catalysts and sensors.

Poster Presentation : **ANAL.P-112**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

SERS-based SARS-CoV-2 assays using gold nanoparticles-encoded M13 bacteriophage networks

Joung-Il Moon, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

We developed a new SERS-based assay platform that can detect severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) with high sensitivity. First, we assembled M13 bacteriophage networks by controlling the concentration of M13 bacteriophage solution. Then gold nanoparticles (AuNPs) synthesized by the citrate reducing method attached to pVIII surface capsid proteins on M13 bacteriophage using thiol-PEG-NHS chemical linker. Finally, AuNPs-encoded M13 bacteriophage networks were deposited on the silicon wafer. When this substrate is exposed to laser light, the incident field is dramatically enhanced at active sites known as electromagnetic “hot junctions” generated by narrow nanogaps between AuNPs on the surface of M13 bacteriophage networks. In this study, a nuclear protein antibody was used as a receptor, and the AuNPs-embedded M13 bacteriophage network was used as a SERS substrate for the sensible detection of SARS-CoV-2. A quantitative analysis of SARS-CoV-2 lysate was performed by monitoring the change in the SERS peak intensity caused by the formation of sandwich immunocomplexes binding between the antibody-conjugated SERS nanotags and the SARS-CoV-2 virion. The results in this study demonstrate the possibility of a clinical application of this SERS-based assay platform that can dramatically improve the detection limit and accuracy of the currently commercialized SARS-CoV-2 assay kits.

Poster Presentation : **ANAL.P-113**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

An integrated metabolomics and transcriptomics study in lung from hamster infected by Covid-19 variant viruses

Sunho Lee, Jueun Lee, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Coronavirus (Covid-19) has been continuously prevalent to the present, and as time goes on, the cycle of appearance of variant viruses causing reduction of the effectiveness of the vaccine and having very strong transmission power is getting shorter. However, pulmonary pathologies associated with the infection of Covid-19 variant viruses remain to be understood on systematic molecular levels.In this study, metabolic profiling was performed using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS) to identify metabolic changes in the Delta and the Omicron variants compared to pre-infection. And then, metabolic profiles of lung samples were integrated with whole transcriptomic profiles of lung samples analyzed by RNA-sequencing.As a result of multivariate analysis, principle component analysis (PCA) score plots showed stronger separation between pre-infection and post-infection in the Delta than the omicron in both metabolomics and transcriptomics analysis.In metabolic profiles, tryptophan metabolism and glutathione metabolism were significantly changed in only Delta group, whereas, histidine metabolism was specifically altered in only Omicron group. These metabolic pathways are known to be involved in inflammatory and immune responses. In addition, we observed many immune response gene ontologies related to corona variant viruses.Transcriptome-metabolite network analysis was performed by infection time in each variant group to investigate systematically changed metabolic pathways. Purine metabolism and arginine biosynthesis were significantly changed in both two groups by up-regulating gene and metabolite levels showing greater increases in the Delta group.These data suggest that the delta variant causes significant inflammation in lung tissue and changes the immune system than the omicron variant by regulating transcriptome and metabolome. This study provides useful information for changes of metabolic pathways affected by Delta and Omicron variants, and these pathways could be therapeutic targets for two covid-19 variants.

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Poster Presentation : **ANAL.P-114**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Trends of PSA proteomes between prostate cancer tissues and blood among 20 cancer patients for early diagnosis

Miseon Jeong, Wonryeon Cho[*]

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Prostate-specific antigen (PSA) is a protein biomarker isolated from the prostate tissue to blood and has been used to screen for prostate cancer (PCa). PSA tests in the blood could raise many false positive diagnoses and then induce follow-up tests such as biopsies which may be unnecessary and potentially dangerous. This study intended to discover the relationship between blood tests in clinics and cancer tissues by determining the PSA ranks in tissue proteomes of PCa patients with different PSA values in their blood for more accurate early diagnosis. The PCa tissues were collected from twenty PCa patients with different PSA values in blood tests. All PCa tissues were homogenized, and proteins were extracted with lysis buffer but detergent. Then each supernatant fluid was trypsin digested and desalted. The proteomes in all PCa tissues were identified and quantified using nLC-MS/MS and protein database search software. The protein ranks in each PCa tissue, including PSA, were determined based on the number of peptides with high confidence levels and protein scores. Then the PSA rank in cancer tissue was compared with the PSA value in each PCa patient's blood according to clinical information.

Poster Presentation : **ANAL.P-115**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Real-time Simultaneous Analysis of Anode and Cathode Exhausts Using In Situ Flow NMR Technique for Investigation of Electrochemical Reaction in Direct Methanol Fuel Cell

Oc Hee Han*, Ryeoyun Hwang[1]

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[1]*Analyzing Science, Chungnam National University, Korea*

Nuclear magnetic resonance (NMR) spectroscopy is excellent for probing electrochemical reactions due to its quantitative and qualitative information. For the in situ simultaneous acquisition of the anode and cathode exhaust spectra, real-time flow-NMR spectroscopy was developed. In the cathode exhaust, the CD3OH from the anode as well as HOD was observed. Ex situ NMR spectroscopy cannot detect gas products because they are lost during sample preparation. On the other hand, the amount of CO2 gas detected in the anode exhaust using our in situ detection method was proportional to the HOD amount. It was also proportional to the cell current generated. Our results show that this in situ real-time analysis could identify and quantify the exhaust components, including the gaseous products. Therefore, our results demonstrate that this in situ real-time analysis is appropriate to study the reaction mechanisms of diverse other liquid-flowing chemical systems in addition to fuel cells. Furthermore, it may be applicable to designing advanced materials.

Poster Presentation : **ANAL.P-116**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Depth Resolved Raman Probe for Remote Measurement of Fat Contents in Milk

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Milk is worldwide consumed product, supplies various nutrients (e.g., Proteins, fats, minerals and vitamins). However, fats from milk can cause increased risk of diseases and also affect obesity development. Accordingly, measuring fat contents of milk is an important issue, and development of its non-destructive and fast analysis method is necessary. Generally, chromatography like GC or LC gives quantitative and qualitative information, but chromatography analysis is expensive, time-consuming, and limited in analysis without opening packaging. That is the reason we select SORS (Spatially Offset Raman Spectroscopy), the most suitable method for analyze without opening package. In this study, we developed method for analyze milk fat without opening package and line-mapping multi-offset Raman Probe system for suppliers, markets and consumers in dairy industry.

Poster Presentation : **ANAL.P-117**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Real-time multi-dimensional single-particle tracking in solution for single-cell dynamcis by intergrated light-sheet-based super-resolution microscopy

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A multi-functional light-sheet-based super-resolution microscopy (LSRM) was investigated by combining with light-sheet, total internal reflection, differential interference contrast, and super-resolution radial fluctuations modules. The cylindrical lens-based astigmatism method was used to determine the spatial movement (x, y, z), while the rotational angles (azimuth and elevation angles) were triggered by orthogonal polarized illuminations. After the surface functionalization of gold nanorods (AuNRs), the motional and rotational behaviors of native AuNRs and functionalized AuNRs in glycerol were studied. This method showed high localization precision of ~6 nm laterally and ~14 nm axially. The results indicated that surface modification of AuNRs largely affected the translational and rotational diffusions in glycerol, which were attributed to the frictional force and van der Waals forces between the AuNRs and glycerol molecules. This technique can be suitable for studying the movement and rotational behavior of surface-modified nanoparticles in solution and single living cells.

Poster Presentation : **ANAL.P-118**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Induced Electrospray Ionization Mass Spectrometry for the Analysis of Metabolites and Proteins at a Single Cell Level

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Department of Chemistry, Dongguk University, Korea

Conventional electrospray ionization (ESI) has been a workhorse for the mass spectrometric analysis of both small molecules like metabolites and biomacromolecules like proteins. However, conventional ESI often suffers from unstable and inefficient spray with a salt-containing sample and undesirable oxidation. In this study, we constructed an induced ESI(InESI) source to partially overcome these issues and investigated the applicability in the analysis of metabolites and proteins at a single cell level. In InESI, alternating current(AC) high voltage(HV) is applied to a sample solution in a non-contacting manner, while direct current(DC) HV is applied by directly contacting an electrode to a sample solution in conventional ESI. With InESI, proteins were found to be less oxidized and form less salt-adduct ions than conventional ESI. Furthermore, InESI enabled more efficient and stable ionization with an extremely small volume(~picoliter) of sample solution than conventional ESI. These features of InESI could ensure highly sensitive analysis with a trace amount of sample solution and thus could be highly beneficial in cell metabolite or protein analysis at a single cell level. Therefore, we tried to obtain single cell ingredients with a microscope-aided cell manipulation system and perform direct analysis of the obtained cell fluid by InESI mass spectrometry(MS). Our results suggest that InESI MS could serve as a highly sensitive and reproducible single cell MS platform.

Poster Presentation : **ANAL.P-119**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Determination and Analysis of Functional Ingredients in Various Forms of Camaecyparis obtusa(Pyeonbaek) Products by Gas Chromatography-Mass Spectrometry

Minjoo Jeong, **Sangwon Cha***

Department of Chemistry, Dongguk University, Korea

Natural complex substances(NCS) of plant origins have been widely used by themselves or as additives to household chemical products. Essential oils are representative forms of NCS and they are often listed in the international organization for standardization(ISO) along with their constituents and contents. However, some of the essential oils we regularly use are not included in the ISO. In case of evaluating the products containing these non-ISO listed essential oils for registration purposes, we face difficulties because it is hard to clearly define the functional components of the corresponding essential oil. In this study, we tried to construct a strategy for determining functional ingredients of non-ISO listed essential oils by employing both text-mining approach and chemical analysis. For this purpose, we selected an essential oil of Camaecyparis obtusa (pyeonbaek) as a model. First, we investigated functional components of pyeonbaek oil and their contents through literature search. Then, we performed quantitative and qualitative analysis of several pyeonbaek oil products by gas chromatography-mass spectrometry (GC-MS). Through this approach, we could determine about ten functional ingredients of pyeonbaek oil. In addition, we also developed and performed chemical analysis for pyeonbaek oil-containing products such as a tooth paste and an oral spray by using direct injection or headspace GC-MS, and evaluated them in terms of contents of determined functional ingredients.

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Poster Presentation : **ANAL.P-120**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Analysis and Differentiation of Citronella Oil by Gas Chromatography and Paper Spray Ionization Mass Spectrometry

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Citronella oil is an essential oil obtained from the leaves and stems of Cymbopogon and has been used widely as a source of scent chemicals in various products such as soap, candles, and incense. Citronella oil also has been known to act as an insect repellent. There are two representative types of citronella oils, Java and Ceylon types, and their constituents and contents are listed in the international organization for standardization(ISO). Chemical analysis of citronella 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 an alternative and fast chemical fingerprinting method by using paper spray ionization MS (PSI MS). PSI utilizes a triangular paper tip for sampling and ionization and enables direct liquid sample analysis with minimal sample preparation. For sensitive detection of functional ingredients of citronella oil including citronellal, citronellol, and geraniol, the parameters for PSI such as spraying solvent composition, spraying voltage, and paper substrate were carefully optimized. We obtained chemical fingerprints from several citronella oil products of two different types by using GC-FID, GC-MS, and optimized PSI MS. Then, chemical fingerprint data obtained from three different analytical platforms were subjected to principal component analysis (PCA) for evaluating the performance of type-differentiation. Through this investigation, we found that PSI MS can serve as a quick and effective tool for differentiating citronella oil products.

Poster Presentation : **ANAL.P-121**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Abiotic Synthesis of Ribonucleosides under Desorption Electrospray Ionization Configuration

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It has been shown that some chemical reactions can be accelerated over 100 to 106 times in microdroplets compared to bulk solution. Reaction acceleration in microdroplets is thought to be accomplished by various factors such as partial solvation, surface-to-area volume increase, reactant confinement, and so on. Recently, abiotic ribose phosphorylation and synthesis of ribonucleosides has been demonstrated successfully in microdroplets generated by electrospray ionization(ESI). In abiotic synthesis of ribonucleosides, the roles of phosphorylated ribose and magnesium ions were highlighted. In this study, we investigated whether ribonucleosides could be synthesized under heterogeneous catalytic environment with magnesium-rich surface. In order to configure this, desorption electrospray ionization(DESI), liquid extraction-based ambient desorption/ionization technique for mass spectrometry(MS), was employed. First, the homebuilt DESI MS interface was tested against the reaction of Girard's reagent T with ketosteroid that has known to be accelerated under DESI MS configuration. After optimizing DESI parameters with a model reaction, studies on the acceleration of ribonucleoside synthesis were conducted. For example, all reactants except magnesium ion were electro-sprayed onto a magnesium-free or -rich surface to investigate the role of magnesium ion in ribonucleoside synthesis. In contrast to the previous report where all reactants were pre-mixed and sprayed, DESI configuration could confirm stepwise reaction by physically separating one reactant from another. Our results suggest that DESI could enable more detailed and precise observation of the mechanism on acceleration of ribonucleoside synthesis occurring in microdroplets.

Poster Presentation : **ANAL.P-122**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation of C-N Bond Formation in Microdroplet Formed by Electrospray Ionization–Mass Spectrometry

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The increasing concentration of carbon dioxide (CO2) in the atmosphere has led to serious environmental issues, making the investigation of carbon dioxide utilization crucial. In this study, we investigated carbon-nitrogen(C-N) bond formation between CO2 and amine compounds in microdroplets as a possible way of carbon dioxide utilization. Reactions in microdroplets have been known to be accelerated due to the surface area to volume ratio increase, the partial solvation, the reagent confinement effect, or the extreme pH condition. In order to realize microdroplet chemistry with CO2, we utilized electrospray ionization (ESI) as a reaction platform and resulting products were monitored in real-time by mass spectrometry (MS). Several methods for direct CO2 introduction into a solution have been tried such as utilization of carbonated water and addition of carbonate/bicarbonate salts into a solution. In addition, since the reaction acceleration in the microdroplet is thought to be often associated with the gas-liquid interfacial environment, we utilized CO2 nebulization gas or dry ice to ensure that the ambient condition surrounding the microdroplets are rich in CO2. We evaluated various CO2-introduction strategies by monitoring production yield of carbamic acids, expecting C-N bond formation products, and tried to determine the critical factors that accomplish accelerated C-N bond formation between CO2 and amine compounds.

Poster Presentation : **ANAL.P-123**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Paper-based Digital Microfluidic Device for Gold Nanorod Synthesis

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Digital microfluidics (DMF) has become an important tool that is useful for a wide range of liquid handling applications. Especially paper-based DMF has emerged as a simple, compact and low-cost method to fabricate fluid manipulation devices. In most experiments, controlling the liquid volume is a critical factor to make the precise concentration of solution. In this study, in order to control the liquid volume precisely we developed a simple micro-dispenser. Integrating it on a paper-based DMF chip, we performed gold nanorod (AuNR) synthesis by varying the concentration, showing the possibility for high precision chemical reactions on lab-on-a chip. For fabrication of the chip, firstly the patterned electrodes were inkjet-printed on photopaper with conductive silver nanoparticle ink. For droplet actuation, the electrowetting-on-dielectric technique was used. Then polysulfone and Teflon, as a dielectric layer and a hydrophobic layer, were spin-coated on the electrodes. This simply fabricated paper-based DMF chip will offer an affordable tool to test various chemical reactions quickly, precisely, and low-costly as well as AuNR synthesis. *Keywords: Paper chip, digital microfluidics, inkjet printing, conductive ink, electrowetting, gold nanorod*

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Poster Presentation : **ANAL.P-124**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Structural studies of Syndecan-4 binding with PIP$_2$ related to signal transduction by NMR

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The syndecan family is transmembrane heparan sulfate proteoglycans (Syndecan-1, -2, -3 and -4) which are composed of a core protein and heparan sulfate found in mammals. Among them, Syndecan-4 plays an important role in the interaction between the extracellular matrix and cytoplasmic signaling molecules and scaffolding proteins. The signal transduction mechanism of syndecan-4 depends on the activity of kinase present in the cytosol. When syndecan-4 forms a complex with PIP$_2$, protein kinase Cα is activated and can control the process of cytoskeleton formation by relocating to the biological membrane and regulating its activity. In this study, when syndecan-4 forms a complex with PIP$_2$, we investigated to identify which residues of syndecan-4 interact with PIP$_2$. Therefore, syndecan-4 with some ecto-domain, transmembrane domain, and cytoplasmic domain sequences was created and named Syd4-eTC. In addition, the oligomerization of syndecan-4 is an important factor in its function. It is known that the GXXXG motif is an important amino acid sequence for oligomerization, therefore, this study indicates the formation of oligomerization by changing this motif in the transmembrane region of syndecan-4.A method for mass production of those peptides was required, so that genetic recombination techniques were used and various analytical techniques such as CD and NMR were used to identify the structure of the peptides. Afterwards, we tried to confirm the interaction with PIP$_2$ through NMR.

Poster Presentation : **ANAL.P-125**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Expression, purification, and structural studies of anti inflammatory tIK peptides

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Rheumatoid arthritis is an autoimmune disease that causes inflammation of the synovial membrane around the joint and destroys ligaments and cartilage. This autoimmune disease is known to be caused by an imbalance between pro-inflammatory and anti-inflammatory cytokines. Recently, it has been found that a specific amino acid sequence of the truncated-IK (tIK) protein inhibits the expression of pro-inflammatory cytokines. However, since the huge molecular weight (29 kDa) of the tIK protein can cause problems such as a significant increase in cost and time required in the pharmaceutical process, we designed some new peptides with short sequences having anti-inflammatory properties based on the tIK protein. Therefore, tIK-9mer, 14mer, and 18mer, which can have anti-inflammatory activity like tIK protein but have small molecular weight, were proposed. Target peptides(tIK series) were expressed by DNA recombinant E. coli and gave rise to high-purity peptides through optimized isolation and purification processes. Since then, the finally purified peptides have been analyzed and studied through various biophysical techniques such as MALDI-TOF, CD, and NMR spectroscopy.

Poster Presentation : **ANAL.P-126**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Comparison of structures between mutant-hMC4R-TM2 and wild type-hMC4R-TM2 through NMR analysis

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Melanocortin receptors (MCR) are members of the rhodopsin family of 7-transmembrane G protein-coupled receptors (GPCR). Especially the human melanocortin-4 receptor (hMC4R) involved in appetite regulation and energy homeostasis. Mutations in the gene in the hMC4R have led to recessive hereditary obesity. Among many mutations, we noted the D90N, a substitution of aspartic acid, the 90th residue to asparagine which is located in TM2. Therefore, we studied by comparing mutant-hMC4R-TM2 (m-hMC4R-second transmembrane domain), with wild type-hMC4R-TM2 (wt-hMC4R-TM2). In order to analyze the structure of the proteins, we obtained pure protein by fast protein liquid chromatography (FPLC). To confirm the structural properties of wt/m-hMC4R-TM2, we applied various spectroscopy methods, including solution-state NMR spectroscopy and solid-state NMR spectroscopy.

Poster Presentation : **ANAL.P-127**

Analytical Chemistry

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Structural study of Amyloid precursor protein’s transmembrane domain using NMR spectroscopy

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Human transmembrane proteins (hTMPs) are involved in many crucial biological processes such as signaling transduction pathways, and the transport of ions and molecules across impermeable membranes. It is very important to identify the structure of the hTMPs to study their function and properties. However, the hydrophobicity of hTMPs makes it more difficult to determine the structure of hTMPs. For this reason, we created a membrane environment to study the structural analysis of hTMPs. Among the many hTMPs, we focused on amyloid precursor protein (APP), which has a relation with Alzheimer's disease (AD).AD is caused by a different APP cleavage system from the normal brain. This difference causes being formed an ion channel that Ca^{2+} permeability in the cell membrane, interrupting calcium ion homeostasis in normal cells. In this study, we made a large-scale highly purified target protein using genetic recombination to confirm the three-dimensional structures of the exact domain from the human APP transmembrane (hAPP-TM) and explain the structure and formation mechanisms of the hAPP-TM channel.We applied HPLC and MS to get and check highly purified protein and used CD and solution-state NMR to analyze the target protein’s secondary structure. Finally, we used solid-state NMR spectroscopy to analyze 3-dimensional alignment in the bicelle environment.

Poster Presentation : **ANAL.P-128**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Structural studies of metal-ion binding to antimicrobial peptides LPcin-YK analogs by NMR spectroscopy

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Abuse of antibiotics has caused severe public health problems, such as the emergence of antibiotic-resistant bacteria. Furthermore, progress of antibiotics has stalled for nearly decades due to the scientific difficulties of developmental research and low economic assessment of antibiotic development. By this reason, it is important to research and develop pharmaceutical substances that can replace antibiotics. Since antimicrobial peptides (AMPs) have a wide range of antimicrobial spectrum and show antimicrobial activity against antibiotic-resistant bacteria, AMPs are highlighted as an alternative to antibiotics. AMPs can penetrate and depolarize cell membranes, and it has a different mechanism of action from conventional antibiotics. Recently, many studies have been conducted on the improvement of antibacterial activity by enhance the penetration of AMPs to cell membrane through metal ion interaction with AMPs. According to this research trend, we confirmed AMPs-metal ion interaction through various spectroscopic techniques.Among the AMPs, we have identified the structure and properties of LPcin-Ⅰ, an antimicrobial peptide found in bovine milk. In many LPcin-Ⅰ analogs, LPcin-YK5, 8, 11 were our main subject. LPcin-YK5, 8, 11 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-129**
Analytical Chemistry
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Method of confirming the purity for DNP(3,4-Dinitropyrazole)

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Agency for Defense Development, Korea

DNP(3,4-Dinitropyrazile) is one of the promising candidates for TNT. Melting point of DNP is similar to TNT. The explosive performance of DNP is better than TNT, Comp-B and higher density than them. Sensitivity to impact, friction, ESD of DNP are insensive. DNP is commercially available starting material and easily nitrated to final product.So we are trying to synthesize the DNP in large scale. Final product remains the acid(nitric acid, sulfuric acid). But there is no specific method of the purity for DNP.As residue of DNP is acid, we propose the acid concentration is analysed by ion chromatography and DSC (Differential Scanning Calorimetry) with high pressure crucible in simple ways. Because of purity of DNP, it might change the thermal property.Here in, the purity of DNP is confirmed by comparing the ion centration, thermal analysis of crude and recrystallized products.

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Poster Presentation : **ANAL.P-130**
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Metal Interface Damping and Refractive Index Effect Study of Single Palladium Coated Gold Nanorods (AuNRs@Pd) Using Dark-Field Microscopy and Spectroscopy

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In this study, we investigated the optical properties of palladium coated gold nanorods (AuNRs@Pd) at the single-particle level using dark-field (DF) method. The AuNRs@Pd were synthesized by in-situ palladium shell epitaxial growth mechanism using CTAB-capped AuNRs, and their structural characterization was carried out by electron microscopes. Afterward, the scattering properties of single AuNRs@Pd were characterized under DF microscopy and spectroscopy. Metal interface damping was observed during the synthesis where the blue-shifting was present during the Pd2+ attachment to AuNR interface. Reduction into Pd induced the red-shifting of the plasmonic scattering spectra. The growth phase of palladium shell alters the peak position due to its aspect ratio changes during synthesis. Localized surface plasmon resonance (LSPR) scattering spectra of the synthesized AuNRs@Pd core-shell showed two broad LSPR peaks at around 624.4(+12.6) nm and 470.8(+1.4) nm that correspond to sub-radiant and super radiant plasmon mode peaks, respectively. Fano resonance was clearly observed as spectral dip at 544.8(+2.9) nm in their single-particle scattering spectra. The plasmon peaks shift were observed in response to refractive index changes, whereas the increment of RI value tends to make both peaks be red-shifted. The position of Fano resonance in response to RI changes is dependent on the thickness of Palladium shell which can bring heterogeneity on LSPR spectrum on each of single nanoparticles. The scattering spectra of thin palladium shell AuNRs@Pd exhibited higher shift sensitivity as a function of refractive index value, where the sensitivity is 2.44 times more on super radiant plasmon peak and 1.55 times more on sub radiant plasmon peak when being compared to the scattering spectra of thick palladium shell bimetallic nanorods.

Poster Presentation : **ANAL.P-131**
Analytical Chemistry
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Layer by Layer Cell Separate, LLCS : Beads Throw Split (BTS)

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This study is to establish an ultra-sensitive quantitative analysis method for tissue layers using Layer by Layer Cell Separate and Liquid Chromatography-Mass Spectrometry (LC-MS) to improve permeability evaluation among chemical/biological active ingredients in human medicines.Medicines are administered to the human body through oral administration, intravenous administration, and mucosal administration. Currently, the drug screening method mainly used is to supply a culture media containing a drug to a target cell in two dimensions, and cannot implement a decrease in drug penetration according to the depth of the tissue with a three-dimensional structure, and accordingly, the drug delivery power can be overestimated. We presented a method using 3D Spheroid, Layer by Layer Cell Separate (LLCS), and LC-MS to improve penetration evaluation through measurement of drug by depth of tissue.In this study, Solid Tumors spheroids will be separated by thickness through Beads Throw Split (BTS) method. The key technology is to break down proteins between and into enzymes, and to separate remaining cell-cell conjugates by using bead. As the bead speed changes depending on the flow rate of the solution and the number of collisions can be adjusted, various conditions such as enzyme concentration, decomposition time, bead type, size, and solution flow rate will be changed to find optimal conditions.With the application of LLCS, the proteins that bind cells between the layers of the spheroids will be broken down and separated without damaging the cells. By using LC-MS to quantify the amount of drug in the extracellular matrix and absorbed in the cell, the permeability and absorption of the drug and target cell can be accurately measured.

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Analytical Chemistry

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A Study on Different Phthalate Extraction Method in Air Samplers by Gas Chromatography/Mass spectrometry (GC/MS)

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Phthalates are representative plasticizers used in various industries, such as electronic products, pharmaceuticals, paints, packaging materials, and so on. Generally, phthalates are measured using extraction methods from samples including liquid extraction, ultra-assisted extraction (UAE) or Soxhlet extraction followed by chromatography. In this study, we compared Headspace Solid Phase Microextraction (HS-SPME) with UAE to extract four phthalates in OVS air samplers. The target phthalates are dimethyl phthalate (DMP), diethyl phthalate (DEP), dibuthyl phthalate (DBP), and bis(2-ethylhexyl) phthalate (DEHP). We optimized the method of HS-SPME for fiber, saturation and adsorption temperatures and time, and desorption temperature and time. As a result, PDMS/DVB fiber, 225℃ saturation and adsorption temperature, 5 min of saturation temperature, 45 min of adsorption time, and 5 min of desorption time were determined as the optimized conditions. For the optimization of the air sampler by UAE, we referred to the conditions from OSHA104 and NIOSH5020 to optimize extraction solvent, temperature, and volume of extraction solvent. The optimized conditions of the UAE were 60℃ extraction temperature with 1 mL of acetone. After optimization processes, both methods were validated, including the limit of detection (LOD), the limit of quantification (LOQ), working range, recovery, sensitivity, and reproducibility. The results obtained from the OVS samplers at different locations showed ND~3,320 ng (DMP), LOD~13,513 ng (DEP), LOD~813 ng (DBP), and 107~1,699 ng (DEHP) using SPME and ND~8,062 ng (DMP), 645~8,165 ng (DEP), ND~4,620 ng (DBP) and 1,244~21,307 ng (DEHP) using UAE. The current UAE method to analyze phthalates from air samplers showed low LOD and LOQ, reasonable recovery, sensitivity, and reproducibility were obtained by UAE method and wide working range by SPME method to analyze phthalates.

Poster Presentation : **ANAL.P-133**
Analytical Chemistry
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Characterization of the size and lamellarity of the vesicles by asymmetrical flow field-flow fractionation coupled online with multi-angle light scattering (AsFlFFF-MALS)

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Vesicles are used in drug delivery systems (DDSs) to encapsulate substances such as proteins and deliver them to a target. These vesicles usually travel by blood vessels to their desired target. During this process, it may be exposed to external stresses such as osmotic pressure caused by the gap in ionic strength between the inside and outside environments. Therefore, the vesicle composed of the lipid bilayer is deformed, and the encapsulated substance does not reach the target, reducing the drug delivery efficiency. It can be used to evaluate drug delivery or encapsulate efficiency by confirming the structural variation of vesicles by osmotic pressure.Vesicles were prepared by the extrusion method under three different ionic strengths of phosphate buffer at pH 7.4. Then, they characterized size, molar mass, shape, and lamellarity using asymmetrical flow field-flow fractionation coupled online with multi-angle light scattering (AsFlFFF-MALS).As a result, the hydrodynamic radius (r_h) was changed from 46 nm to 41 nm, and rms radius (r_g) was changed from 56 nm to 47 nm with an increasing gap of ionic strength (I) between inside and outside (ΔI = 40 mM).In addition, lamellarity was determined by comparing the vesicle's experimental and theoretical molar mass. From this result, we monitored that the hypo-osmotic environment forms more multilamellar vesicles than the iso-osmotic environment while forming more multilayers in the hyper-osmotic environment for small-sized vesicles.

Poster Presentation : **ANAL.P-134**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Uncovering Key Domains for Amyloid-*β* (1-42) Fibrillar Aggregation: Implications for Therapeutic Interventions

Dongjoon Im, Dongvin Kwak, Da Gyeong Hyun, Gyusub Yoon, Yeonjeong Kim, Sehyun Hwang, Hugh I. Kim[*]

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Many neurodegenerative diseases have clinical signs that are fibrillar amyloid aggregates. One of the main components of senile plaques in the brains of people with Alzheimer's disease is the amyloid-*β* (1-42) protein, making it a key target for disease therapy. The development of aggregation inhibitors as possible therapeutic medicines depends critically on identifying the key domains of amyloid-*β* (1-42) that enable its oligomerization. In this work, we found three important hydrophobic domains on amyloid-*β* (1-42) and looked into their role in the protein's self-assembly. Based on these discoveries, we created potential amyloid-*β*(1-42) aggregation inhibitor peptides. Utilizing the developed peptides, we investigated the functions of the three hydrophobic domains during amyloid-*β* (1-42) fibrillar aggregation and observed the ensuing impacts on its aggregation behavior and structural conversion. Also, we looked at the interactions between the two C-terminal end residues and the two hydrophobic domains, as well as their functions in amyloid self-assembly, using an amyloid-*β* (1-42) double point mutant (I41N/A42N). Our findings suggest that the central hydrophobic region of amyloid-*β* (1-42) has interchain interactions that are crucial for fibrillar aggregation, and that these interactions affect how accessible the central hydrophobic area is to the start of the oligomerization process. Our research identifies important structural domains that aid in the self-assembly of amyloid-*β*(1-42) and offers mechanistic insights into how it occurs. These findings can also be used to enhance the rational design of potential amyloid-*β*(1-42) aggregation inhibitors.

Poster Presentation : **ANAL.P-135**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation of dual-targeting natural product inhibitors on amyloid protein aggregation

Da Gyeong Hyun, Dongjoon Im, Dongvin Kwak, Gyusub Yoon, Yeonjeong Kim, Sehyun Hwang, Hugh I. Kim*

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Alzheimer’s disease (AD) is a type of neurodegenerative disease that leads to cognitive dysfunction and memory loss. Senile plaques and neurofibrillary tangles (NFTs) are considered pathological hallmarks of AD, which are generally observed at the interior and exterior of the nerve cells of AD patients. These pathogenic amyloid aggregates are generated by misfolding of amyloid-β (1-42) (Aβ42) and tau proteins, respectively. Thus, several types of research were suggested to discover therapeutic approaches for AD by suppressing the formation of pathogenic amyloid aggregates including small molecules, post-translational modification (PTM), monoclonal antibodies, and rationally-designed peptide inhibitors. However, despite to approval of monoclonal antibodies including Aducanumab and Lecanemab by the U.S. Food and Drug Administration (FDA), the efficacy was still controversial. Therefore, alternative therapeutic strategies against AD are required. Natural products are a type of small molecule, containing compounds and metabolites obtained by living organisms. Most of all, genipin and pyrogallol were noticed as potential therapeutic candidates against AD due to their abilities to alleviate oxidative stress and neuroinflammation. Herein, we discovered the potential of genipin and pyrogallol to suppress amyloid protein aggregation through multidisciplinary biophysical analyses. The compelling results suggest the applicability of genipin and pyrogallol as therapeutic agents against AD by revealing the underlying molecular mechanisms suppressing amyloid protein aggregation.

Poster Presentation : **ANAL.P-136**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

An Efficient Chemical Analysis Method for Secondary Batteries using LDI TOF-MS and the Battery MS Database

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Lithium-ion batteries are among the most promising energy storage device due to their high energy density. Despite their many advantages, lithium-ion batteries do have some limitations that need to be addressed. One of the major challenges is the risk of fire or explosion, which can occur if the battery is damaged or exposed to high temperatures. To address this issue, researchers are developing new materials and technologies that can improve the safety and reliability of lithium-ion batteries. In addition, researchers are also exploring new analytical techniques that can provide more detailed information about the behavior of lithium-ion batteries at the molecular level, but there are not many technologies that can observe composing elements or molecules and identify their distribution directly. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) is a powerful surface analysis technology for batteries, but it is limited to interpret the molecular information from the complicated spectrum due to the strong energy of ion beams. On the other hand, Laser Desorption Ionization Time-of-Flight Mass Spectrometry (LDI TOF-MS) provides more informative mass spectra including relatively less fragmented and more molecular structural information due to its relatively soft ionization process. In addition, we are also exploring the use of LDI TOF-MS for high-resolution mass imaging of nano-scale electronic devices, including lithium-ion batteries and OLEDs. To reduce the analysis time of LDI mass spectra and make them more accessible for various field applications, we are also developing battery MS databases that can be used for fast and convenient interpretation of the complicated mass spectra. These databases can help researchers to identify and characterize the various components of a battery, including the cathode, anode, and electrolyte, and to monitor changes in the composition of the battery MS database are promising tools for battery analysis, and they have the potential to provide valuable insights into the behavior of lithium-

ion batteries at the molecular level, which could lead to the development of even better battery materials and technologies in the future.

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Poster Presentation : **ANAL.P-137**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

PPIAT: Target Mass Spectrometry-based Protein-Protein Interaction Analytics Tool

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The formation of protein networks and protein complex structures through protein-protein interactions (PPIs) is crucial for understanding the biological functions of proteins. Many human diseases result from abnormal PPIs involving endogenous proteins, proteins from pathogens or both. In other words, understanding protein-protein networking not only allows for an understanding of disease mechanisms, but also improves our understanding of protein structures and functions. Cross-linking mass spectrometry (XL-MS) is a powerful method that has been developed over several decades to map PPIs. However, it has been hindered by several key obstacles, including searching for theoretical protein interactions, identifying actual interacting regions between proteins, and calculating mass values. Furthermore, there is a shortage of analysis tools available for mapping PPIs. Generally, targeted mass spectrometry-based XL-MS method is performed by profiling a target protein and the proteins that interact with it, based on MS/MS values. However, the highly complex fragmentation of actual interacting peptides and the lack of analysis tools remain major impediments to efficient research. While various analysis tools are used in combination to map and analyze PPIs, these tools are not integrated, and all cases where protein interactions are theoretically possible must be known in advance.To overcome these hurdles, we suggest using PPIAT. PPIAT is a web-based analytics tool that utilizes STRING and UniProt databases to search for theoretical interacting proteins for target proteins and calculate their mass in peptide and ion level, taking into consideration all possible interactions with each protein complex. Additionally, the results calculated from PPIAT can be summarized and extracted based on the probability score of protein interaction in the derived results and other analysis tools such as Prego, and can be used as input data for target mass spectrometry analysis.

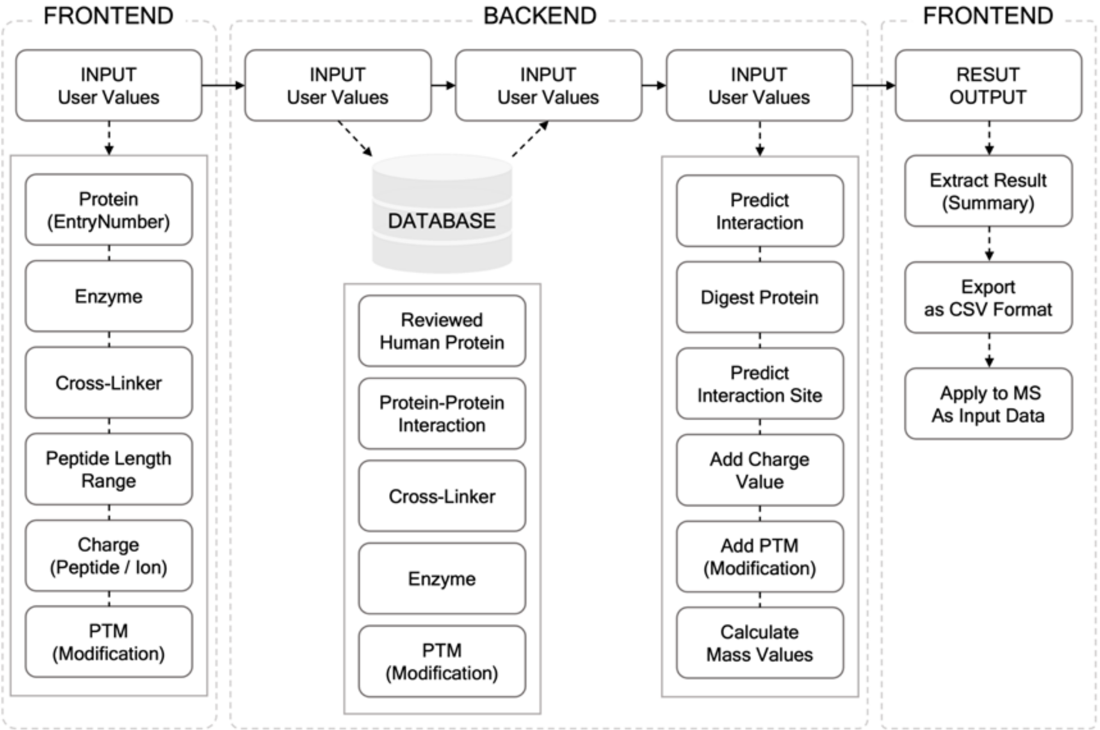

Fig. 1| Workflow of PPIAT The figure presents the flow of the PPIAT. Information for searching protein-protein interaction(PPIs) is input at front-end. Data queried from database by input information at front-end and PPIs and each mass value are calculated considering input condition. All calculated data presents at front-end and the result can export as CSV format. The exported data can use as input data for MS/MS analysis.

Poster Presentation : **ANAL.P-138**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhanced Detection and Quantitation of Brain-derived Glycolipids using LC/MRM-MS-based Platform

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Glycolipids enriched on cell membrane microdomains play significant roles in signal transduction, neuronal cell recovery, differentiation, and memory. Experimental evidence for quantitative changes of specific glycolipids in various neurological diseases such as Alzheimer's disease, Parkinson's disease, and epilepsy strongly supports the importance of glycolipids in brain disease pathogenesis and potential treatment. Therefore, analytical methods for absolute quantitation of disease-related target glycolipids are essential for biomarker discovery and disease monitoring. However, glycolipids are amphiphilic substances consisting of a hydrophilic carbohydrate chain and a hydrophobic ceramide moiety, which makes their separation and analysis extremely challenging. Here, we developed a highly sensitive and highly selective absolute quantitation platform based on reversed-phase LC/MRM-MS. First, the organic modifier content of the diluent was increased to improve the solubility of glycolipids, which directly affects data repeatability. We also optimized the ratio of isopropanol in the mobile phase solvent to enhance the instrument repeatability and minimize the increase of column pressure due to isopropanol. As a result, we could determine high sensitivity analysis at the femtomole level and achieve high repeatability within 8% of the CV. The calibration curve was quantitatively linear with a correlation coefficient (R^2) greater than 0.99. This analytical method enables the detection of ng levels of glycolipids per µg of protein in brain tissue. Our glycolipid quantitation platform will be utilized with a high potential for diagnosis and monitoring of glycolipid-related diseases.

Poster Presentation : **ANAL.P-139**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Alginate Characterization Strategy through Absolute Monosaccharides Quantification utilizing PMP Labeling and LC/MRM-MS

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Alginic acid, which is widely used in various industries such as food, biomedicine, and pharmaceuticals, is a polysaccharide derived from cell walls of brown algae. Alginate is composed of randomly arranged hexuronic acid residues β-D-mannuronic acid(M) and α-L-guluronic acid(G) with 1,4-glycosidic linkages. Recently, it has attracted attention as a new functional biomaterial as it has been found to exhibit various biological activities such as antioxidant, antitumor, and immunomodulatory. Nevertheless, elucidating the relationship between structural properties and biological function remains challenging due to the lack of tools to characterize alginate. Here, we introduce an alginate characterization strategy through simultaneous absolute quantification of 14monosaccharides commonly found in nature based on LC/MRM-MS. Monosaccharides with isomeric structures were baseline separated and monitored via PMP labeling and structure-specific ions produced by MS/MS. This method allowed us to obtain the most important information about alginate: the ratio and purity (i.e. content) of M and G. In fact, 14monosaccharides could be successfully absolute quantified from attomole to femtomole in alginate extracted from seven species, which are brown algae in Korea. As a result, we determined that the extracts derived from various brown algae contained more than 60% of alginate, among which M/G ratio was 1.7 for Ecklonia cava and 2.5 for Ishige okamurae. Ultimately, our analytical platform and results will serve as a useful reference for understanding the structure and properties of alginate.

Poster Presentation : **ANAL.P-140**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation and Design of Nitric Oxide via Electrochemical Platform with COMSOL Simulation

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Nitric oxide (NO) is one of the gaseous messenger molecules that has played crucial biological roles via interacting directly and reversibly in multiple biological systems, such as cardiovascular homeostasis and the immune system. The NO signaling pathway is known to proceed by reacting NO with the iron containing haem prosthetic groups in the soluble guanylyl cyclase (sGC) or with thiol groups in cysteine protein (S-nitrosylation) to trigger a conformational change. [7] It also reacts with reactive oxygen species (ROS) and thiol groups in biomolecules, causing DNA damage or inhibiting metabolism. In order to control the amount of NO generation precisely, developments of various NO-releasing platform has been studied. And among them, it was necessary to conduct an analysis on whether the design of the platform would be done as we intended. This was done through COMSOL Multi-physics, and the calculation was used together with the Cd and Tds modules. We enhanced the spatiotemporal understanding of the NO generating platform through simulation.

Poster Presentation : **ANAL.P-141**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Thermofluidic Consideration in Nanoplastics Detection using Surface-Enhanced Raman Spectroscopy

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As interest in nanoplastics (NPs) increases, various detection techniques have been suggested. Among them, surface-enhanced Raman spectroscopy (SERS) has received a lot of attention because it provides the information of molecular fingerprints with outstanding high sensitivity. On the other hand, it is known that the laser irradiation used in SERS measurement causes a plasmonic heating effect in the local hot spot area on the surface. However, such heating effect has not been considered together with the thermofluidic properties of nanoplastics during the measurements. Here, we systematically examined such heating effects by using standard type of polystyrene (PS) and polymethyl methacrylate (PMMA) nanoparticles which are deposited on a well-controlled SERS surface. Dark field spectroscopy allows the optical visualization of individual particles, where laser was irradiated with controlled power density. We showed that nanoplastics can be locally melted on the SERS surface with increasing laser power, verifying the permeation of nanoplastics into a hotspot. Our results suggest that when measuring nanoplastics by SERS, factors such as laser power, plastic type (different melting temperature) and SERS substrate property should be considered all together.

Poster Presentation : **ANAL.P-142**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Novel analytical strategy for investigating the pH of individual atmospheric aerosol particles

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Aerosols are a micrometer-sized particulate matter suspended in the atmosphere that affects climate change and human health. The pH of aerosol particles plays a crucial role in regulating gas-particle partitioning, phase separation, and the heterogeneous reactions that produce secondary organic and inorganic components. Understanding the pH of individual aerosol particles is essential because they exist and behave independently, yet it has been challenging due to the absence of suitable analytical technique. This study provides a novel analytical strategy for the investigation of pH of individual aerosol particles based on the surface-enhanced Raman spectroscopy (SERS). While SERS has been demonstrated to be an effective tool for investigating aerosol pH, this is the first application of SERS to the investigation of individual aerosol particles. A SERS-active substrate suitable for investigating the pH of individual aerosol particles was fabricated using the silver-mirror reaction and subsequently functionalized with 4-mercaptopyridine (4-MPY) to act as a pH indicator. Aerosol particles in a size range similar to that of ambient atmospheric aerosols were nebulized on the SERS-active substrate using a home-made aerosol nebulizing system. SERS measurements were conducted in an in-situ measurement setting that stabilized relative humidity to maintain the water content of individual aerosol particles. The results of this study demonstrate the successful distinction of aerosol particles with pH ranges of 1-7 using standard solutions, indicating the suitability of this approach for analyzing ambient aerosol particle pH. Further studies are ongoing, focusing on the characterization of individual aerosol particle pH with respect to size, time, and relative humidity.

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Poster Presentation : **ANAL.P-143**
Analytical Chemistry
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Development of Volatile Organic Compounds (VOCs) Analysis device in Exhaled breath using TD-GC/MS

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Exhaled breath testing is becoming an increasingly important diagnostic method that canbe used in the evaluation of health and disease states. It has the advantage of being simple and quick to test compared to other tests. About 3,000 types of VOCs are included in the breath exhaled by humans, but 20 to 30 of them are used as biomarkers for diseases. In the study, a low cost and simple device was developed to measure VOCs in respiration. The subject held their breath for the first 5 seconds and repeated the process of inhaling and exhaling at intervals of 3 seconds for 5 minutes. The exhaled breath is carried through the tube and from the tedlar bag to the TD tube via the pump. The pump, temperature sensor, and fan in the device are all controlled by Arduino. The sampling TD tube is analyzed through TD-GC/MS and can be used as a biomarker of a disease by identifying a substance that appears in a specific disease.

Poster Presentation : **ANAL.P-144**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Multiplexed detection of pathogens using barcoded-hydrogel microparticles

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MicroRNAs (miRNAs) regulating gene expression can be used as biomarker for various disease like cancer and neurodegenerative disorders. However, reverse transcription PCR, conventional approach for miRNA detection, has its drawback in multiplexed detection capabilities because it requires sophisticated probes and multiple channel in equipment that cause complexity and high cost for detecting various targets. To overcome these problems, we introduced barcoded-poly(ethylene glycol) diacrylate (PEGDA) microparticles and isothermal exponential amplification reaction (EXPAR) that can be used for detecting pathogens in multiplexed manner. Not only miRNA, but antibodies are immobilized on microparticles, being used as sensors for detecting various bacteria. Furthermore, barcoded-microparticles are integrated with microwell system to partition samples and conduct digital EXPAR.

Poster Presentation : **ANAL.P-145**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Isolation and identification of soil microorganisms that biodegrade Polybutylene Adipate Terephthalate(PBAT)

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Plastics are polymeric carbon polymers, which are largely divided into non-biodegradable and biodegradable. Non-biodegradable plastics are widely used around the world, and the accumulation of used plastics is causing a lot of environmental pollution. In order to solve this problem of plastic waste, biodegradable plastics are being developed as an alternative. Among them, polybutylene adipate terephthalate (PBAT) is a petroleum-based biodegradable plastic that uses terephthalic acid and is known to biodegrade within 6 months. In this study, microorganisms that degrade PBAT in soil were isolated, identified and investigated to understand its' action mechanism. Pre-treatment processes are also studied and optimized to accelerate bio-degradation by UV-exposure, chemical-treatment and physical pre-process. Micron-thickness PBAT film was produced by spreading-method and it was buried in compost to isolate PBAT-decomposing microorganism for 30, 60, 90 and 180 days. Films were then analyzed with SEM to image degradation rate and microorganisms in the film surface. Films were also characterized with FT-IR, NMR, TGA and DSC to understand degradation mechanism. PBAT-degrading microorganisms were colonized to separate each species and they were identified through 16s rRNA analysis.

Poster Presentation : **ANAL.P-146**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a Sophisticated Lab Automation System via 3D Printer Modification

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This study aims to present a sophisticated lab automation system that entirely automates the sample preparation process for liquid chromatography/mass spectrometry (LC/MS) through the modification of a 3D printer. The system streamlines several intricately organized sample pretreatment procedures, including micro pipetting, gripping, vortexing, centrifugation, and heating block shaking, with no human intervention required. The automation system comprises three modular subsystems: an automated liquid handling system (ALHS) that automates the sample preparation process, an automated storage and retrieval system (ASRS) that stores and retrieves samples, laboratory consumables, and modularized experimental instruments, and an automated transport system (ATS) that transports objects between ALHS and ASRS. Each subsystem is modular in design, allowing for easy integration and optimization for users. All the necessary information for the creation of the system, such as design files, assembly manuals, and software, is made available to the public as an open-source resource.

Poster Presentation : **ANAL.P-147**
Analytical Chemistry
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Analysis of Carbazole-based molecule distribution in solar cells using Orbitrap/TOF Hybrid SIMS

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Analysis of the chemical structure of a multi-layered solar cell is very important in terms of correlation with power conversion efficiency. TOF-SIMS is a powerful analytical tool for device characterization due to the following advantages; wide analysis range from insulators to organics, excellent detection limits (~ppm). However, TOF-SIMS is of limited use in the analysis of organics with high mass values due to its relatively low mass resolution and difficulty in interpretation due to its relatively low mass resolution and difficulty in interpretating numerous mass peaks. It is often analyzed in an indirect way, for example by observing small ions such as $–NH_2$, -CN contained in a molecule. To overcome this, the depth behavior of carbazole-based conjugated organic molecules (CzxN) included as electrolytes in solar cells was studied using high-resolution Orbitrap/TOF Hybrid SIMS. Specifically, we designed a systematic approach that can accurately analyze the depth behavior of an actual intact molecule by accurately finding the characteristic peak of the molecule of interest through the principal component analysis (PCA) method and verifying the chemical structure by performing MS/MS analysis. Through this study, we present a new analysis method that can obtain clear chemical information about molecules of interest included in multi-layer thin film devices such as solar cells and OLEDs by overcoming the limitations of conventional TOF-SIMS.

Poster Presentation : **ANAL.P-148**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Intramolecular C-N Bond Formation on Immobilized Au NPs in a Microchamber Reactor

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Nitrogen-containing organic compounds are extensively found in bioactive natural products and pharmaceutical materials, and those materials have been highlighted the importance in the pharmaceutical market and electronics industry. While much effort to construct the intramolecular C-N bond formation has been continued, C-N bond formation under mild condition is still a challenging task for organic synthetic chemists. Various groups have conducted amination reactions using transition metal catalyzes like Pd, Cu, and Ru in the past decades. However, those protocols still have inevitable problems that use high temperatures, toxic solvents, long reaction times, and so on. Organic reactions using photocatalysts could be one alternative strategy to overcome inherent issues in conventional C-N bond formation. In most photocatalytic systems, the reactions were conducted in a colloidal system containing nanocatalysts. In such cases, the transfer of charge carriers generated in nanocatalysts by light absorption is limited due to a relatively long migration distance between donors and acceptors, and the intensity of transmitted light gradually decreases in accordance with the penetration length in a reactor. In this work, we demonstrated intramolecular C-N bond formation in a “house-built” microchamber type reactor and the amination of aminobiphenyl was chosen as a model system. The reaction efficiency between the colloidal system and the microreactor was evaluated as well. The nanocatalysts and products were characterized using TEM, GC-MS, NMR, and Raman spectroscopy.

Poster Presentation : **ANAL.P-149**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Chiral Au Nanostructures and Applications to Raman Analysis

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Chirality is a term for "asymmetry", a geometrical property of structures in which an object and its mirrored image cannot be superimposed. Chirality is one of the most important basic concepts in sciences such as biology, chemistry, and physics, and this property can be used in many fields, such as chiral sensors and displays. Natural molecules respond to ultraviolet, but it is difficult to apply to biosensing or biomedical fields because the intensity of chiroptical responses shown in the ultraviolet is weak. On the other hand, chiral nanostructures can provide strong chiroptical responses in the visible and infrared regions due to the strong plasmon resonance of nanostructures. Therefore, if chirality is given to established nanostructures, they can be used in more fields along with nanophotonics and optoelectronic devices. In this study, we synthesized nanoparticles using the seeded growth method and imparted chirality to the nanoparticles using organic molecules with chirality in the process of growth. Several chiral nanoparticles were finally synthesized using various chiral organic molecules and by controlling the shapes of seed particles. The morphologies of chiral Au nanostructures were characterized with TEM and SEM, and the optical properties of chiral nanostructures were confirmed by CD. Furthermore, we performed SERS analysis to investigate the shift in Raman scattering of organic molecules depending on the chirality of Au nanostructures.

Poster Presentation : **ANAL.P-150**
Analytical Chemistry
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Visible-Light-Active TiO_2-Cu@Ag Photocatalyst Nanocomposite for Degradation of dye and Inactivation of Bacteria and Fungus(*Staphylococcus aureus* and *Candida albicans*)

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Bacterial infections are one of the greatest threats to global human health. That is why antibacterial technology continues to be researched. In the present study, TiO_2, which is the original UV-activated photocatalyst material, was doped with Cu to shift the photoactive range to the visible light range, and Ag doped to increase the bioavailability. During Visible-Light-Active treatment, TiO_2-Cu@Ag Nanocomposites are excited by light with a visible light wavelength in the presence of oxygen, leading to the production of reactive molecular species (RMS). RMS could kill bacteria by oxidatively damaging their biomolecules, especially those constituting the external structures of bacteria, such as the cell membrane and cell wall. Visible-Light-Active Inactivation of bacteria about TiO_2-Cu@Ag nanocomposites is tested by CFU assay that is analytical method for checking the number of bacterial cells in a solution. As a result, TiO_2-Cu@Ag nanocomposite showed some inactivation of two strains (*S. aureus* (bacterium) and *C. albicans* (Fungus)) of five strains tested under visible light. Therefore, although TiO_2-Cu@Ag Nanocomposites was found to exhibit some antibacterial activity under visible light, but was confirmed to reveal not specifically identified bacterial specificity. If the mechanism for the killing of bacteria and fungi is identified in detail, it can be used as another antibacterial technology.

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Poster Presentation : **ANAL.P-151**
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Highly Sensitive and Label-Free Detection of Influenza H5N1 Viral Proteins Using Affinity Peptide and Porous BSA/MXene Nanocomposite Electrode

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Influenza viruses can cause pandemics through animal-to-human and inter-human transmission. Neuraminidase (NA), a glycoprotein on the surface of influenza A and B viruses, is a promising candidate for testing due to its minor immunogenicity. We used phage display to identify an affinity peptide specific to the influenza H5N1 virus NA, which was assessed for its binding affinity via enzyme-linked immunosorbent assay (ELISA). Four synthetic peptides were chemically synthesized and tested to develop an affinity peptide-based electrochemical biosensing system. Among the peptides tested, INA BP2 peptide was selected as a potential candidate and subjected to square wave voltammetry (SWV) for evaluating its detection performance. To enhance the analytical performance, we applied a three-dimensional porous bovine serum albumin (BSA)–MXene (BSA/MXene) matrix. The surface morphology of the BSA/MXene film-deposited electrode was analyzed using X-ray photoelectron spectroscopy (XPS), field-emission scanning electron microscopy (FE-SEM), and electrochemical measurements (CV and EIS). The BSA/MXene nanocomposite-based peptide sensor showed a significant dissociation constant (Kd = 9.34 ± 1.20 nM) and a low limit of detection (LOD, 0.098 nM) using SWV measurement. The sensor exhibited good reproducibility, stability, and recovery, even in the presence of human plasma. Our study demonstrates a new bioanalytical sensing platform for developing highly sensitive virus detection methods.

Poster Presentation : **ANAL.P-152**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of the solvent free headspace GC-MS analysis method for the detection and quantification of benzyl chloride Impurities in drug products

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Various genetically toxic chemical impurities are commonly present as by-products in the production of synthetic drugs prescribed for the treatment of various diseases. Active pharmaceutical ingredient (API) manufacturers must develop ways to effectively manage these impurities and perform thorough verification before launching the deployment. Benzyl chloride is a representative carcinogen used in the synthesis process of various drugs, and various studies have been conducted. In this study, a solvent-free headspace gas chromatography-mass spectrometry (SF-HS-GC/MS) method was developed to detect benzyl chloride to the low parts-per-billion level. The experimental conditions of the solvent-free headspace system were optimized using the culture temperature, time, and sample amount parameters. The SF-HS-GC/MS method verified linearity, quantitative limit (LOQ), precision, and accuracy, in accordance with the Q2(R1) ICH guideline and ICH M7, and introduced samples in split mode with DB-5MS UI column (30 m x 0.25 mm, 0.25). The calibration curve ranges from 0.05 to 5 μg/g, with a correlation coefficient exceeding 0.9998 and a LOQ of 0.1 μg/g. Precision %CV was less than 5% and accuracy was between 95 and 105%. In addition, the formation of benzyl chloride under headspace conditions was confirmed in various drugs, and benzyl chloride was not confirmed. The developed method can be used as a guideline for screening and detection of benzyl chloride in APIs and pharmaceuticals.

Poster Presentation : **ANAL.P-153**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Highly sensitive label-free electrochemical biosensor for detection of C-reactive protein

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C-reactive protein (CRP) is an acute plasma protein that appear in the human bloodstream. The level of CRP increase in inflammatory conditions and cause diverse inflammatory disease. Current biosensors for CRP detection require a significant long time, and cost expensive. In this study, we developed a novel peptide-based platform of label-free electrochemical biosensors for rapid and selective detection of CRP. To improve the performance of the sensors, black phosphorus dispered with AuNPs were incorporated onto the peptide sensor layer. The interaction between CRP binding specific peptide and CRP were confirmed by electrochemical analyses and molecular docking system, and the developed sensors were characterized by enzyme-linked immunosorbent assays (ELISA), X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscope (FESEM) and several electrochemical analyses. Under the optimized conditions, the peptide-based sensor incorporating AuNPs@BP@PDA showed a good binding affinity in a wide range of 0-0.036 μg/mL with a detection limit (LOD) of 0.923 ng/mL for CRP detection. The results obtained from the electrochemical analyses of the serum and plasma samples of patients suffering from Crohn’s disease with developed our sensor showed an acceptable accuracy. Thus, the fabricated peptide-based biosensors has potential application for clinical diagnostics with a highly rapid and sensitive detection of CRP.

Poster Presentation : **ANAL.P-154**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Sample Preparation Methods for Liquid Chromatography Tandem Mass Spectrometric Analysis of Ingredients in Household Chemical Products

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Recently, there has been increased concern regarding exposure to unknown hazardous chemicals in household chemical products (HCPs). However, there is a limitation to identify unrevealed ingredients in HCPs with a single analytical method due to their diverse physicochemical properties. Suspect screening analysis using liquid chromatography–mass spectrometry (LC-MS) is an effective technique to identify polar compound in HCPs. In this study, we developed a sample preparation method for HCPs and identified uncovered ingredients in the products.The following three types of HCPs were selected for the present study according to the product formulation: aerosol, water-soluble liquid, and water-soluble powder type. Basic condition solid phase extraction (SPE) using 0.02% ammonium hydroxide solution was performed to remove anionic surfactants in HCPs. Extracted samples were analyzed using a UHPLC-Q-TOF mass spectrometer, and chemicals were identified using NIST 20 MS/MS spectral library. As a result, fatty acids showed decreased intensity in the basic condition SPE compared to acidic SPE. Suspect screening analysis revealed unknown seven compounds across the tested HCPs, which were matched against commercially available reference standards. For the confirmed chemicals, recovery tests were performed using matrix matched calibration methods.The developed sample preparation method can provide knowledge of unknown hazardous chemicals in HCPs.

Poster Presentation : **ANAL.P-155**
Analytical Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Toxicological Effects of Microplastic Fibers from Different Disposable Face Masks on Soil Nematodes

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

Since the COVID-19 outbreak, disposable masks have been widely implemented as a primary preventive measure to minimize virus transmission. Despite their high usage, there has been limited research on the impact of disposable masks on soil ecosystems. This study aims to investigate the toxicological effects of microplastics from masks on Caenorhabditis. elegans (C. elegans) in the soil media. The toxic effects of microplastics from three types of disposable masks (KF94 mask, medical mask, and particulate respirator) and a polypropylene (PP) reference material on the growth and number of offspring of C. elegans were evaluated. The results showed that the growth of C. elegans was not affected by microplastic exposure. However, significant decrease in the number of C. elegans offspring were observed in KF94 masks and particulate masks when exposed to 0.3% (microplastics/soil, w/w) microplastics. Mass spectrometry-based metabolome analysis revealed distinct metabolic changes between the masks, which were not detectable in phenotype. Alterations in the polyamine biosynthetic pathway, which is involved in reproductive function in C. elegans, were commonly observed in the KF94 mask and particulate respirator exposed groups. On the contrary, the pattern of quantitative changes in metabolites was not identical in the two groups. Analysis of mask extracts using ultra-high resolution MS revealed plastic additives that can be reproductively toxic to C. elegans, such as phthalates, suggesting that various plastic additives may be responsible for reproductive toxicity in C. elegans.

Poster Presentation : **ANAL.P-156**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Quantitative Proteomic Analysis of Human Neutroblastoma Cells Exposed to Particulate Matter

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Particulate matter (PM) is known to be an environmental risk factor that gives rise to deleterious effects on human health. Owing to its chemical components (e.g., polycyclic aromatic hydrocarbons, NO2, SO2, and so on), inhalation of PM might cause diverse diseases, such as, cardiovascular, respiratory, eye, and skin diseases. Until now, PM studies have generally been focused on the circulatory and respiratory systems. In this study, an effect of PM on the nervous system was investigated using PM exposed neuroblastoma cell (SH-SY5Y). Proteins obtained from PM exposed SH-SY5Y were compared with those from normal SH-SY5Y to obtain biomarker candidates. A global quantitative proteomic analysis of two SH-SY5Y samples was performed using isobaric tags for relative and absolute quantification (iTRAQ) based 2D nano-liquid chromatography-electrospray ionization-tandem mass spectrometry. We confirmed that proteins related to neural development were reduced and those related to cell death were increased due to PM exposure.

Poster Presentation : **ANAL.P-157**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Investigation of enzymatic oxidation mechanism of model lignins using LC-ESI-MS/MS

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There are growing demands for the valorization of lignin into depolymerized aromatic chemicals. In our previous work, enzymatic oxidation using laccase, a multicopper oxidase, was reported to produce valuable benzaldehyde chemicals from plant lignin, but the mechanism of transformation remains unknown. To understand the mechanism of laccase-mediated oxidation of lignin, the oxidation products of lignin model dimers with three different linkage types (G(8-O-4)G, G(8-5)G, and G(8-8)G) were characterized using liquid chromatography-electrospray ionization-tandem mass spectrometry coupled with a UV detector for selective detection of aromatic chemicals. Under laccase treatment for 24 h, 69%, 61%, and 89% of G(8-O-4)G, G(8-5)G, and G(8-8)G model dimers were transformed into oxidation products, respectively. The abundance of an aldehyde-functionalized oxidation product (m/z 713.2595, 2(G(8-5)G+CH2O)) of G(8-5)G was increased six times compared with the control sample without enzyme treatment, whereas the abundances of aldehyde-functionalized products of G(8-O-4)G and G(8-8)G were unchanged. MS/MS spectrum of the aldehyde-functionalized oxidation product (m/z 713.2595, 2(G(8-5)G+CH2O)) revealed the neutral losses of two aldehyde groups (CH2O and 2CH2O, m/z 30.01 and 60.02). Collectively, these results suggest that the enzymatic transformation of lignin into benzaldehyde chemicals could be associated with the oxidation of (8-5)-type lignin linkage.

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Poster Presentation : **ANAL.P-158**
Analytical Chemistry
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Fabrication of Cobalt Nanoparticles with Controlled Morphology as Electrocatalyst for Water Splitting

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The formation of transition metal nanoparticles (NPs) has been extensively studied due to their high surface-to-volume ratio compared to bulk catalytic materials. Metal NPs of different size and shapes have different crystallographic facets and have different fraction of surface atoms on their corners and edges, which makes it interesting to study the effect of metal nanoparticle shape on the activity of various reactions. Especially, some of transition metal nanoparticles are useful in several processes due to their magnetic properties. The synthesis of transition metal NPs involves the reduction of metal ions in solution, typically using a reducing agent, a stabilizing agent, and a solvent. The size, shape, and structure of the resulting NPs can be controlled by adjusting the reaction parameters, such as the concentration of the metal precursor, the type and amount of reducing agents and the reaction temperature. In this study, we synthesize various cobalt nanoparticle and size by liquid phase reduction. Scanning electron microscope, transmission electron microscope, and X-ray diffraction are used to characterize the synthesized NPs. Effect of the size and shape of the nanoparticles for OER activities we are investigated using various electrochemical technique.

Poster Presentation : **ANAL.P-159**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Multipods Silica for SERS-active Substrate Application by Gold Coating

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Recently there have been significant research interests in the design of plasmonic metal nanoparticle structures due to their unique optical and electrical properties dominated by the collective oscillations of free electrons in the metal, known as surface plasmons. Plasmonic metal nanostructures with unique geometric nanostructures can amplify surface-enhanced Raman scattering (SERS) signals by generating strong localized surface plasmon resonance and hot spots. We synthesized multipods silica nanoparticles in a one-pot method which has many bumps on the particle surface. The multipods silica nanoparticle's shape had affected by sodium halide ions. We made gold-coated multipods silica nanoparticles and investigated their surface morphology and SERS effect using scanning electron microscopy and Raman spectroscopy. Further, the finite element method (FEM) simulation (COMSOL Multiphysics 5.6, Waveoptics Module) showed a higher signal in the electric field of the gold-coated multipods silica nanoparticle. Our study, thus, demonstrates that the gold-coated multipods silica nanoparticles can be used as potential SERS-active substrates for various diagnostic and sensing applications.

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Analytical Chemistry
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Fabrication of Uniform Gold Nanorods (Au NRs) Using Modular Microfluidic Device

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‘Seed-meditated method’ is a widely used method for synthesizing gold nanorods (Au NRs). In the method, Au seed particles having a size of 2-3 nm are synthesized and then grown into Au NRs in a growth solution. However, it is reported that due to the high reactivity of the reducing agent, uniformly reacting within the reactor when using the batch reactor is difficult, and thus the uniformity of the synthesized Au seed is low. To solve this problem, we fabricated Au seeds using a continuous flow microfluidic module chip reactor. It significantly reduces the time required for material and heat transfer and the distance required for diffusion between materials due to the high surface area-to-volume ratio at a microscale. These features enable a uniform and very fast reaction within a reactor. In addition, the 'modular' microfluidic system has the advantage of being able to easily control experimental conditions such as mixing points by assembling various individual chips that each play a different role.Therefore, a continuous flow reactor was constructed using a 'modular microfluidic device', and the size, uniformity, and reproducibility improvement of the synthesized Au seed by adjusting the relative injection flow rate of the reducing agent and buffer solution and surfactant was conducted. Buffer solution was used for control reactivity of the reducing agent. TEM and UV-vis analysis were conducted to confirm the size and uniformity of the synthesized Au seed. And adding a growth step after the Au seed synthesis, process of nanorods growth will be analyzed in a real-time using flow cell type modular chip

Poster Presentation : **ANAL.P-161**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Highly Sensitive 3D SERS-Active Substrate with Abundant Hot Spots for Detection of cTnI Biomarkers

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Immunoassays using surface-enhanced Raman scattering (SERS) for biomarker detection have become an active research field due to their high sensitivity and selectivity. In this study, 3D SERS-active substrate with abundant hot spots was developed for the detection of biomarkers. Nickel foam with a three-dimensional(3D) structure provided a large specific surface area. SERS substrate with hot spots was formed by gold deposition after making nanostructures with surface modification through thermal. As a result, we were able to detect MGITC, Raman reporter, at a very low concentration(10e-10 M), indicating the high sensitivity and reproducibility substrate. In addition, we conducted a competition assay using 50 nm-sized gold nanoparticles and 3D SERS-active substrate, and the limit of detection of cTnI was determined to be 1 pg/mL. The 3D SERS-active substrates with abundant hot spots have the potential to be used as a sensitive and selective tool for the detection of various biomarkers in complex biological samples.

Poster Presentation : **ANAL.P-162**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Dielectrophoretic Control of Plasmonic Metal Nanoparticle onto The Patterned Substrate for SERS-Active Substrate

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Dielectrophoresis (DEP) induces dipoles to cause movement of particles. When a polarizable particle is placed in a non-uniform electric field, a dipole is induced due to the non-uniform electric field, resulting in a force imbalance at both ends. In DEP, it is essential to generate an electric field gradient, and the method mainly used is to fabricate a unique type of electrode. We will fabricate a SERS active substrate with uniformly arranged particles by applying DEP to plasmonic metal nanoparticles. Plasmonic metal nanoparticles have a unique phenomenon called LSPR, which is caused by the collective oscillation of electrons on the surface, and SERS arises from this phenomenon. Since LSPR occurs more strongly in a nanogap called a hotspot between nanoparticles and a metal structure, it is important to generate many hotspots to induce the SERS effect. In addition, since a uniform structure with a uniform nanogap is required, the particles must be uniformly arranged. However, it is very difficult to arrange the nanoparticles uniformly. Therefore, we will fabricate a SERS active substrate for molecular detection by inducing particle motion using DEP and arranging them to have a constant nanogap.In this study, gold-coated silica nanoparticles and patterned silicon substrates are used. The silicon substrate has regularly arranged circular patterns and is coated with a thin gold film due to the low conductivity of silicon. In DEP, particles having a diameter of about 800 nm were used because the larger the volume of the particle, the more sensitive it is to DEP. And it was confirmed that a relatively strong electric field gradient was formed at the edge of the cylindrical pattern through FDTD simulation (COMSOL Multiphysics, AC/DC Module).

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Analytical Chemistry

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Fabrication of Porous Polymer Shell on Carbon Sphere and Application for Catalyst

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Photocatalysis is a promising technique with many applications, such as renewable energy production and treatment of environmental pollution. Titanium dioxide is one of the most widely researched photocatalyst, but has low efficiency and narrow light response range. So, combining titanium dioxide with porous carbon materials can enhance photocatalytic activity due to many advantages such as high surface area, large pore volume, accessible interior spaces. As a result, porous shell on carbon sphere can be applied to the photocatalyst with good performance. In this study, we synthesized mesoporous polydopamine coated resorcinol formaldehyde carbon (RFC) nanoparticles. First, a facile method fabrication RFP sphere with from 100nm to 600nm in diameter has been successfully achieved via sol-gel process which can control particle size. Second, we can be obtained porous nanoparticles coated porous polydopamine shell. Third, we fabricated porous polydopamine shell on carbon sphere by converting polymer into carbon through calcination. Consequently, due to porous polydopamine shell, it can be used as a photocatalyst by forming a nanocomposite with titanium dioxide and applied as a catalyst support in various fields by using various metal oxide.

Poster Presentation : **ANAL.P-164**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Upconversion Nanoparticles with Controlled Morphology for Plasmonic Enhancement of Optical Property

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Upconversion nanoparticles (UCNs) consist of hexagonal NaYF4 nanocrystals doped with trivalent lanthanum ions, which absorb low-energy radiation to release higher energy radiation. UCNs with hexagonal phase are the useful structure for emitting strong photoluminescence (PL). In this study, rod-shaped UCNs with hexagonal phase were synthesized and phase transition can be controlled by adjusting the ratio of gadolinium. When the ratio of gadolinium is more than 30 percent, pure hexagonal phase is observed because the effect of phase transition is greater than that of particles growing. UCNs with 30 percent gadolinium have the highest PL intensity because they have the highest phase homogeneity and the largest size. Plasmonic metal nanoparticles have collective oscillations of free electrons on their surface called localized surface plasmon resonance (LSPR). Their integration can improve the fluorescence of the phosphor by the incident electromagnetic field enhancement arising from LSPR. However, quenching effect reduces fluorescence by nonradiative energy transfer. In this study, we coated the mesoporous silica shell using the synthesized UCNs. The thickness of the silica shell was grown to reduce the quenching effect. We synthesized mesoporous silica shell to increase the surface area. Also, attaching plasmonic metal nanoparticles on mesoporous silica-coated UCNs to enhance the plasmonic effect is ongoing.

Poster Presentation : **ANAL.P-165**

Analytical Chemistry

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Fabrication of Mesoscopic Star-Shaped Gold Particles as SERS-active Substrate

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SERS(Surface-enhanced Raman Spectroscopy) is a highly sensitive molecular detection technique that enhances Raman scattering of molecules adsorbed on metal nanoparticles or nanostructures. Recently, major efforts have been made to synthesize precious metal nanoparticles of various sizes and shapes, which can control surface plasma resonance (LSPR). Complex geometrical structures with numerous sharp projections show LSPR scattering peaks at multiple wavelengths of direction and polarization. In gold meso-star synthesis, a three-step seed-mediated chemical method can give a high-yield synthesis of gold meso-star. Without silver nitrate, irregular and uncontrollable shapes of gold particles are formed. But when silver nitrate is added at the end, we can synthesize star-shaped gold microparticles with numerous sharp tips on their surface due to silver ions’ effect on multi-directional growth, and they can generate strong local field enhancement. The more hot spots are formed by the Localized Surface Plasmon and the larger the particle size, the SERS signal increases. Gold meso-stars have strengths in both factors, so they can be used in various fields such as bio-molecular sensing. We have arranged gold meso-star particles to patterned substrates and then investigated whether they can be used as a highly sensitive SERS-active substrate.

Poster Presentation : **ANAL.P-166**
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Facile Fabrication of Titanium Dioxide Nanoparticles Encapsulated inside Multi-Walled Carbon Nanotubes and Its Application for Photocatalyst

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A facile method fabrication multi-walled carbon nanotubes (MWCNTs) with titanium dioxide nanoparticles has been successfully achieved via solid state reactions. In the previous study, nanocomposites of titanium dioxide particles encapsulated inside multi-walled carbon nanotubes were fabricated and characterized by basic analysis such as transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM). Also, adsorption and decomposition experiments of organic materials were performed to characterize the photocatalytic performance of the fabricated nanocomposites. In this study, additional photocatalytic disinfection experiment was performed. E. coli and MS2 coliphage were used as hazardous materials to be removed, and both showed excellent removal rates. Also, a recycling experiment was performed to confirm repetitive catalyst reusability of the nanocomposites, and an ESR analysis was performed to confirm reactive oxygen species (ROS).

Poster Presentation : **ANAL.P-167**

Analytical Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of 3D heterostructured MOF-derived B-doped Cobalt/Cobalt-oxide@N-doped carbon for effective alkaline water-splitting activity

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The sluggish oxygen evolution reaction (OER) at the anode and hydrogen evolution reaction (HER) at the cathode in alkaline media demands high overpotentials for water-splitting which require high-cost catalysts like Pt and IrO2/RuO2, etc. In this regard, low-cost transition metal-based electrocatalysts, especially those derived from the metal-organic framework (MOF) present a new class of high-performance electrocatalysts due to their unique physicochemical properties. In this study, freestanding and 3D mesoporous heterostructures of Cobalt/Cobalt-oxide@N-doped carbon with tunable Cobalt valence states hybridized in N-doped carbon matrix on a metal foam substrate were developed through a facile synthesis route, and evaluated for OER, HER, and overall alkaline water-splitting activities. The electrocatalysts showed excellent bifunctional electrocatalytic activities demanding low overpotentials and excellent stability for 50 h.

Poster Presentation : **LIFE.P-168**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Novel Design of Phase Separation Drivers Based on Fluorescent Proteins

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Liquid-liquid phase separation (LLPS) of biomolecules has recently attracted broad interest due to its role in the spatiotemporal compartmentalization of eukaryotic cells. Two types of proteins are known to drive phase separation: multi-domain proteins and intrinsically disordered proteins (IDPs). Multi-domain proteins are composed of folded domains connected by disordered linkers, and LLPS of multi-domain proteins is driven by the interactions between the folded domains. Previous research has mostly focused on IDPs, due to the overwhelming number of biological examples, and few are known for LLPS of multi-domain proteins. In this work, we propose a new design of multi-domain proteins that drive LLPS and use the new system to investigate the molecular principles behind LLPS of multi-domain proteins.We constructed dimers and trimers of widely used fluorescent proteins, yellow fluorescent protein (YFP), green fluorescent protein (GFP), and mCherry, and utilized metal-histidine coordination chemistry as a means to increase valency. Upon the addition of metal ions, immediate phase separation was observed under a fluorescence microscope. We quantitatively determined the saturation concentration by turbidity measurement and checked the liquidity of droplets using the fluorescence recovery after photobleaching (FRAP) assay. The effects of domain binding affinity, metal ion, and crowding agent (polyethylene glycol) have been investigated. We suggest that our system is suitable as a minimalistic model for investigating the molecular principles of phase-separated proteins.

Poster Presentation : **LIFE.P-169**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

NMR study on the interaction of human ADAR1 with Z-DNA and Z-RNA

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Human ADAR1 deaminates adenosine in pre-mRNA to yield inosine, which codes as a guanine residue in mRNA. ADAR1 edits dsRNA in vitro at significantly higher levels when dsRNA contains the purine-pyrimidine repeats that could easily form a left-handed Z-RNA helix. Human ADAR1 deaminates adenine in pre-mRNA to yield inosine (I), which codes as a guanine residue in mRNA. These A-to-I conversions can lead to functional changes in the resulting proteins. The Zα domains of human ADAR1 (ZαADAR1) bind to Z-DNA via interaction mediated by the α3-core and β-hairpin. Five residues in the α3 helix and four residues in the β-hairpin play important roles in Zα function, forming direct or water-mediated hydrogen bonds with DNA backbone phosphates or interacting hydrophobically with DNA bases. 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. Comparison of these results provides the structural information to explain the origin of Aicardi-Goutières syndrome.

Poster Presentation : **LIFE.P-170**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Target DNA recognition of human transcription factor HoxA1 using NMR

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In humans, the Hox genes are distributed into four linkage groups, HoxA, HoxB, HoxC, and HoxD, which locate on chromosomes 7, 17, 12, and 2, respectively. HoxA1 is thought to be involved in the placement of hindbrain segments in the proper location along the anterior-posterior axis during development. Homeodomain (HD) protein has 60 amino acids which are highly conserved in α1 and α3 helices. The N-terminal arm (L1) and loop regions (L2 and L3) between the helices are also well conserved. Interestingly, the second and third residues in L1 loop are conserved as the positive charged residues, Lys(K) or Arg(R), among almost all Hox proteins. However, the HoxA1 has residues Asn(N) and Ala(A) in position 2 and 3 instead of K and R. In order to understand molecular mechanism of DNA recognition of HoxA1, we have performed NMR experiments on the homeodomain of HoxA1 (HoxA1-HD) complexed with 10-bp consensus DNA 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.

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Life Chemistry

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NMR study of Transciption Factor DLX3 and Its DNA Recognition

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Transcription factors refer to a protein that binds to a specific site of DNA to promote or inhibit gene expression. DLX3 protein consists of amino acids 1 to 287. Among them, the homeodomain part, known to bind to DNA, is 129-188. A mutation in DLX3 Homeodomain cause TDO syndrome. Highly conserved DLX3 recognizes a common sequence motif, 5'- TAATTG-3'. In this study, DNA and DLX3 protein complex was found as molecular mechanisms of specific DNA recognition through 2D HSQC in NMR. We present the binding affinity of the DLX3-HD for DNA at various salt concentration conditions. This experiment provides structural features of the DLX3-DNA complex and the mechanism of target DNA recognition of DLX3 transcription factors. And we are going to study four mutations that cause TDO syndrome.

Poster Presentation : **LIFE.P-172**

Life Chemistry

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Discovery of phthalazinone derivative as an ENPP1 inhibitor for STING-mediated Cancer Immunotherapy.

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cGAS (Cyclic guanosine monophosphate (GMP)–adenosine monophosphate (AMP) synthase)-STING (stimulator of interferon genes) pathway plays an important role in activating innate immunity. 2’3’-cGAMP, a natural ligand of STING, is synthesized by cGAS. 2’3’-cGAMP promotes secretion of Type Ⅰ interferon cytokine by activating STING downstream pathway and tumor infiltration of cytotoxic T lymphocytes. Recently, research that explores STING-targeted immunotherapy has been studied extensively. However, the bioavailability of STING agonists is limited due to lots of limitations. Thus, we intend to present a new modality for immunotherapy by focusing on the ENPP1 enzyme that degrades 2’3’-cGAMP. In this study, cpd x as a selective ENPP inhibitor was developed to enhance the activity of both intra and extracellular cGAMP. We confirmed that cpd x inhibits the degradation of 2’3’-cGAMP and enhances Type Ⅰ interferon responses and the activation of STING pathway in both host immune cells and tumor cells. In addition, it has the advantages of pharmacokinetics and plasma stability, so oral administration was possible. Finally, results from the in vivo study showed powerful inhibition of tumor growth in a syngeneic CT26 colorectal cancer mouse model and induction of immunological memory that protected against tumor re-challenge. Our result proposes a promising anti-cancer drug that is orally bioavailable as well as induces excellent anti-cancer effects by linking innate immune and adaptive immune.

Poster Presentation : **LIFE.P-173**
Life Chemistry
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Relationship between tubulin inhibitors and STING-IRF3 signaling pathway

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Cancer immunotherapy, which activates the human immune system and lets immune cells selectively remove cancer cells, has been significantly developed and successfully enhanced the prognosis of patients. However, there are emerging needs for next-generation cancer immunotherapy since most patients do not show reactivity to immune checkpoint inhibitors such as PD-1 and CTLA-4. Cyclic GMP-AMP synthase (cGAS)-stimulator of interferon genes (STING) pathway, which is a natural mechanism for sensing foreign DNA to regulate cellular response, has been introduced as a new way to induce interferon-mediated innate immunity and anti-cancer effects. In this study, the random library screening was performed to find compounds that show a synergic effect to 2’,3’-cyclic GMP-AMP (2’,3’-cGAMP), a natural ligand to STING protein. We have found that each selected hit compound had similar structures to several tubulin inhibitors. Therefore, the relationship between tubulin inhibitors and the activation of the STING pathway was investigated, mainly by showing the synergic effects of tubulin inhibitors and 2’,3’-cGAMP. This study showed the role of tubulin inhibitors in the activation of the STING pathway and the newly introduced possible mechanism of bypassing TBK1 and phosphorylation of IRF3 during the progress of the STING pathway.

Poster Presentation : **LIFE.P-174**

Life Chemistry

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Observing Nanoscale Deformation of Actin in Human Dermal Fibroblasts using Super-resolution Microscopy

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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 strecth 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-175**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a non-invasive oral prodrug targeting β-galactosidase in senescent cells for the treatment of age-related macular degeneration

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A common treatment for age-related macular degeneration is to inject it into the eye finer than the hair. This treatment method causes fear in the patient because the needle is visible, so we try to develop an oral prodrug to reduce the patient's fear. Oral drug delivery has many advantages, including high patient compliance, low cost, and ease of use. Based on these advantages, we are trying to develop a new oral prodrug for the treatment of age-related macular degeneration (AMD). To develop new oral drugs that can maintain toxicity while linking specific linkers to existing drugs that are too toxic to senescent cells to increase selectivity. In retinal pigment epithelial cells within AMD, the prodrug can function as a drug that can be specifically cleaved and used by enzymes overexpressed in aging cells. The β-galactosidase protein overexpressed in AMD is a hydrolase that can be used as a biomarker for aging and catalyzes hydrolysis only in aged cells. Therefore, we are trying to develop a new oral prodrug N201-gal that can be cleaved by β-galactosidase proteins that target aging retinal pigment epithelial cells. N201-gal travels through the mouth, stomach, and internal organs to blood vessels and reaches the eyes. Finally, in the senescent retinal pigment epithelial cells of the eye, N201-gal can kill aging cell lines as a highly toxic drug when converted to N201. As a result, new oral prodrug N201-gal, that can deliver an N201 drug cleaved by the β-galactosidase protein from macular degenerated cells to kill aging cells.

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Construction of fluorescent protein expression system to study intramolecular interaction of protein kinase C isoforms

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Activation and inactivation of protein kinase C (PKC) isoforms in mammalian cells control various signaling pathways including cell proliferation, differentiation, and apoptosis. There are at least 10 PKC isoforms in mammalian cells with overlapping and distinct functions. Different PKC isoforms are known to be expressed depending on tissue types. All of PKC isoforms have regulatory domain for cofactor binding and catalytic domain for substrate phosphorylation. Activation of PKC isoforms requires binding of specific cofactors and phosphorylation by other kinases in isoform-specific manner. PKC isoforms also have pseudosubstrate sequences in the regulatory domain. PKC isoforms have been reported to maintain their inactive states by binding between regulatory domain and catalytic domain through pseudosubstrate sequence. We generated various fluorescent protein expression system to study intramolecular interaction between regulatory domain and catalytic domain using fluorescence resonance energy transfer (FRET) in vivo and in vitro. Bacterial expression systems for Cerulean, YPet and Cherry were generated using pET28-based expression vectors. Expression systems for YPet-mCerulean, YPet-mCherry were also generated for FRET positive control. Fluorescent proteins were expressed in BL21(DE3) E.coli strain and tested for fluorescence induced by excitation light (365nm). Histidine-tagged fluorescent proteins were also purified by Ni-NTA column.

Poster Presentation : **LIFE.P-177**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Untangling Pathways of RNA Hairpins in Gaseous Phase Investigated using Ion Mobility Spectrometry-Mass Spectrometry

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RNA hairpins are an essential secondary structure in RNA molecules, playing a significant role in RNA folding, mRNA protection, and recognition by RNA-binding proteins. These structures are formed and stabilized by relatively weak, rather than covalent, hydrogen bonds between the bases in RNA. The process of dissociation of these hydrogen bonds and the subsequent untangling of the structure can reveal important properties of RNA, such as the melting curve in general. In this study, we investigate the untangling pathways of RNA hairpins through charge-charge repulsion in order to uncover their hidden characteristics. We compare the disentanglement of four RNA sequences that are expected to form the same hairpin structure in solution, but with different base pairs, using a stepwise charge addition approach. Overcharging of RNA in the gas phase may result in the breaking of hydrogen bonds or the unfolding of the bent structures. The collision cross-section (CCS) obtained from electrospray ionization (ESI) and ion mobility spectrometry-mass spectrometry (IMS-MS) provide a subtle distinction between hydrogen bond cleavage and structural unfolding. The experimental results of the charge-dependent untangling of hairpin structures offer valuable insight into the overall stability of small RNA.

Poster Presentation : **LIFE.P-178**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhancement of Cell-Extracellular Matrix and Cell-Surface Interactions in Mammalian Cells through $\alpha_5\beta_1$ Integrin Overexpression

Albertus Ivan Brilian, Sang Ho Lee, Kwanwoo Shin*

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In the field of 3D cell and organoid assembly, the interaction between cells and their microenvironment, such as the extracellular matrix (ECM), is a crucial factor in the successful self-organized growth of cells in vitro. Recent studies have demonstrated the pivotal role of $\alpha_5\beta_1$ integrin and soluble fibronectins in cell-ECM force generation and ECM polymerization. To enhance cell-ECM interaction, we overexpressed α5β1 integrin in human dermal fibroblast (HDF) cells using recombinant lentiviruses. The resulting α_5 and β_1 overexpressed cells were selected using the G418 selection method to establish a stable cell line, which was then analyzed for α_5 and β_1 expression using western blotting. The results showed that overexpression of integrin altered the phenotype of the HDF cells, including size and proliferation rate, and resulted in an increase in ECM proteins such as fibronectin and collagen. The enhanced interaction between cells and their environment observed in the integrin-overexpressed cells can be utilized to construct ECM-rich 3D cell assemblies.

Poster Presentation : **LIFE.P-179**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Research on spatial confinement and crowded environment for cytoskeletal networks of actin and microtubules

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The cytoskeleton including actin filaments, microtubules and intermediate filaments play a role in different types of cells and cellular shape and motility through their dynamic interaction with their own unique morphological features. The main of this biopolymer networks are actin networks and microtubules networks, whose generation and mechanical and dynamic properties are highly distinct, thus researches in cell and in vitro are very hard and complicate because of a large mechanical parameters space, crowded components and various cross linkers. Yet how actin networks and microtubules networks affect generating each other, are affected on spatial confinement and crowded components is still unclear. So, in simplification of “synthetic cell” approaches, we have done the researches on spatial confinement and crowded environment for the physical interaction and differences of morphology between microtubule-actin filaments networks and fibers networks made by using divalent cation (Mg ions) without cross linkers. In case of microtubules, we could see the generation of fibers networks under even 5 mM of Mg ions, but actin fibers networks were generated on over 30 ~ 40 mM of Mg ions, that is the concentration of critical threshold of Mg ions for generating actin fibers networks. For actin filaments networks, we could see on the confinement space as small droplets of 20 ~ 200μm diameter under critical threshold of Mg ions for actin fibers networks. Microtubule fibers networks showed different morphological changes depending on the height scale to hundreds of μm between two glass plates from tens of μm like small droplets than the actin fibers networks. Also, microtubules fibers showed results that are greatly affected by the crowded environment. In contrast, actin showed a confinement effect only at a scale of several tens of μm, as in a very small droplet. These results will provide us some understanding of the influences of spatial confinement and crowded components for formation and interaction of actin and microtubules filaments networks or fibers networks.


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Poster Presentation : **LIFE.P-180**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Structure-activity relationship study of a small molecule that synergistically activates the STING pathway with cGAMP

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One of the third-generation cancer therapies, immune checkpoint inhibitors have shown effective anti-tumor effects. However, in some solid tumors, immune cells cannot function properly due to the tumor microenvironment. Therefore, targeting immune cells towards tumors is a crucial issue, and one of the keys to solving this problem is the activation of the STING(Stimulator of interferon genes) protein. When the STING-cGAS pathway is activated, immune-activating signaling molecules called INF signals are transcribed, inducing immune responses in the cell. Using a combination of the STING-cGAS pathway and immune checkpoint inhibitors can result in an effective anti-tumor effect. We identified a substance that enhances STING activation when processed together with cGAMP, and conducted a SAR study to find a more dramatic effect.

Poster Presentation : **LIFE.P-181**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Redirection of CAR-T Cell Cytotoxicity using Metabolic Glycan Labeling with Unnatural Sugars

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T cells expressing chimeric antigen receptors (CAR-T cells) have shown unprecedented clinical responses against hematological malignancies. However, some patients relapse after CAR-T cell therapy due to antigen-negative escape variants. Additionally, CAR-T cell therapies showed limited clinical efficacy in solid tumors with high antigen heterogeneity. To overcome this, we metabolically labeled the glycans on cancer cells to redirect CAR-T cell cytotoxicity regardless of the endogenous antigen expression status of the cancer cells. From in vitro assays and in vivo prophylactic xenograft models, we found that modifying cancer cells with ManNAz and BCN-FITC can elicit selective and durable cytotoxicity of anti-FITC CAR-T cells, whereas less efficient cytotoxicity was elicited by modification with GalNAz and BCN-FITC. Furthermore, we demonstrated that a sialic acid derivative conjugated with DNP hapten (Sia-DNP) generated DNP-modified glycans on cancer cells in situ that could be effectively targeted by anti-DNP CAR-T cells to eradicate established tumors in xenograft models. Our study illustrates that metabolic glycan labeling using unnatural sugars can be combined with targeted CAR-T cell therapy to provide novel cancer immunotherapy for solid tumors that lack viable target antigens.

Poster Presentation : **LIFE.P-182**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Improve ‘click to release’ reaction by modification of tetrazine molecules.

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With the advancement of click chemistry technology, new strategies have been introduced that can be utilized not only for the ligation of two molecules but also for the lysis of bioconjugates. The bioorthogonal cleavage reaction, also known as 'click to release,' is an exceptional tool for in vivo applications due to its biorthogonal nature and fast-occurring characteristics. Despite these advantageous characteristics, 'click to release' does not always achieve complete release, and the need for a faster rate still exists. To address this unmet need, we are working on modifying tetrazine molecules to serve as triggers for 'click to release', with the aim of improving their release rate and yield.

Poster Presentation : **LIFE.P-183**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Artificial photosynthetic organelles using novel rhodopsin operating in extreme environment.

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Photosynthesis is the most important energy-generation mechanism for the survival of living being among many energy systems. And photosynthesis is a system used by plant or other organisms to convert light energy into chemical energy. Microbial rhodopsin was primarily used to develop a photosynthetic artificial organelles that generate energy by mediating light from the past. Previous research has shown how much ATP is synthesized and how many proton gradients the organelles created by proton reconstitution create, but the research of efficiency and stability of membrane proteins in the artificial cellular membranes still need to be further improved. Here, we present an artificial organelle constructed with a novel microbial rhodopsin, tara76 microbial rhodopsin, and demonstrate that it can operate in extreme environments in order to improve reconstitution efficiency. The tara76 rhodopsin is more stable at extreme pH and temperature environments than other rhodopsins and has higher proton pumping efficiency than bacteriorhodopsin (BR) and proteorhodopsin (PR), which were commonly used in previous research. To confirm the efficiency of tara76 rhodopsin in the artificial cells, we constructed small unilamellar vesicles(SUVs) and giant unilamellar vesicles(GUVs) using the detergent-mediated method. We also measured the pH of expression of microbial rhodopsin and proton pumping efficiency by pH indicator dye, Carboxyl SNARF-1, and directly measured with pH meter in the rhodopsin reconstituted liposome condition to confirm the activity of tara76 rhodopsins in the articial cells on extreme pH and temperature environments. This approach might offer the best method for building different transmembrane functionalities in the artificial cell model and allow for the creation of bio-inspired vesicle systems. Also, understanding photosynthesis using this artificial cell can be point the way to improve various understanding the origin of life and energy application.

Poster Presentation : **LIFE.P-184**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Oxidized membrane proteome behind the photocatalytic initiation of non-canonical pyroptosis

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Pyroptosis, a pro-inflammatory programmed cell death, has drawn attention of researchers for therapeutic applications such as cancer immunotherapy. Although a pathogen-like stimulus can be utilized for its initiation, a chemical inducer of pyroptosis based on rational molecular design is required for future therapeutic optimizations. Herein, we propose a photocatalytic cycle of a donor-acceptor type organic molecule, BTP, can trigger pyroptosis through non-canonical pyroptosis. BTP catalysed oxidation of water for Label-free proteomics revealed broad oxidation of membrane proteins leading to maladaptive UPR and accumulation of misfolded proteins that are related with pyroptotic cell death.

Poster Presentation : **LIFE.P-185**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Analyzing the interaction between phospholipid membrane and the antibiotic using artificial cell

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The artificial cell is a vesicle that mimics the specific system of the live cell. Because artificial cells contain only the desired metabolism, they can conduct independent research on specific chemical reactions, molecular recognition, material transport, and energy conversion. Among them, GUV is commonly used to study the biological function of cells because the size of GUV is similar to that of a cell. The antibiotics we used are a test version of a drug that has been shown to have antibacterial effects in cell experiments. However, it is difficult to determine the exact cause of cell death through cell experiments. According to many researchers, most antibiotics cause cell death through membrane modification. In this study, we use GUV as a bio-reactor to observe the independent reaction between the cell membrane and the antibiotics and to analyze the mechanism of these drugs' cell membrane modification. Two variables are chosen for this study. The charge of the phospholipid is used to determine whether the interaction is caused by an electric force, and the concentration of the drug is used to determine the tendency of interaction. Through this research, we expect that artificial cells will be able to propose a new type of analysis that can detect the individual reaction between the specific cell system and the drug.

Poster Presentation : **LIFE.P-186**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Cell-free Protein Synthesis Using Cell Lysate in Giant Unilamellar Vesicle

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An approach to understanding living things through construction is the bottom-up assembly of synthetic cell systems that can replicate biological functions. To create artificial cells, which can translate information in enclosed microcompartments and are separated from the outside environment by a membrane, are typically generated under out-of-equilibrium conditions. These two characteristics are essential for preventing biomolecule diffusion and, more crucially, allowing development to occur through biological evolution. In this research, giant unilamellar vesicles (GUVs) are generated and used as artificial cell membranes to encapsulate the energy molecules, unnatural amino acids, plasmid DNA, cell lysate, and other essential biomolecules as transcription-translation machinery for synthesis target proteins such as green fluorescence protein (GFP). The GUVs made by the emulsion transfer method (ETM), in which water-in-oil emulsion passed through a monolayer at the oil-water interface and then created a phospholipid bilayer by centrifugation. Finally, we successfully synthesized GFP in GUVs, and the intensity of GFP increased steadily with time. The lysate-based system is reasonably priced compared to other extremely expensive systems. The cell-free protein synthesis system based on cell lysate could be encapsulated in GUV to form a model for a sustainable artificial bioreactor, which is essential for synthetic membrane protein in the future and be applied in drug delivery.Keywords: artificial cell, giant unilamellar vesicle, emulsion transfer method, cell lysate

Poster Presentation : **LIFE.P-187**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Extracellular-matrix proteins alters lipid distribution observed on artificial cell model

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Lipid rafts are microdomains of the plasma membrane composed of a specific lipid composition and protein content. While the existence of lipid rafts is widely accepted, the factors that regulate their formation, size, and structure are still an active area of research, with various hypotheses and models being proposed and debated. Nevertheless, research into lipid rafts continues to shed light on their crucial role in cellular function and to reveal new insights into their dynamic nature. Recently, several factors have been identified that influence the distribution of lipids on the plasma membrane. In addition to the well-known interaction between sphingomyelin and cholesterol, mediated by hydrogen bonds, there is a diverse array of lipid-protein interactions that contribute to the formation of lipid rafts. Particularly, some transmembrane has higher affinity to cholesterol, some proteins can form covalent bonds with membrane lipids and the size of the proteins shows effects on the size the raft. In addition to membrane proteins, cytoskeleton proteins such as actin can also participate in the formation of lipid rafts through their associated receptors at the plasma membrane. However, the role that extracellular matrix (ECM) proteins, which interact with the membrane from the outside, play in lipid raft formation remains an open question. We constructed an artificial cell membrane model composed of simplified and controlled components to directly observe the distribution of lipids in the cell model in response to lipid interactions. Different types of ECM proteins altered lipid distribution in distinct ways. However, in general, binding of ECM proteins stabilized lipid domains by retarding their diffusion upon heating. The underlying mechanism was partially elucidated through Fluorescence Recovery After Photobleaching (FRAP) measurements, which quantify the difference in diffusion rates between ECM-bound and free lipid domains. This study contributes a novel insight into the identification of factors that influence lipid raft formation and properties.


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Poster Presentation : **LIFE.P-188**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

PCR-based Nuclear Model Synthesis Inside of Artificial Cell

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To understand life phenomena, many researchers tried to understand and study cells using artificial cells. To mimic the function of living cells, it is necessary to have the ability to replicate and translate genes inside synthetic cells and even perform metabolic processes. DNA replication and transfer of amplified DNA into and out of the vesicles are necessary for all processes to occur. Therefore, we amplified the DNA inside of vesicles and release amplified DNA to out of vesicles. The emulsion transfer method was used to encapsulate DNA and other chemicals inside the vesicles, which were blocked from the outside by phospholipid double membranes. Shuttle PCR (2 temperature) was used instead of traditional PCR (3 temperature) to prevent bursting of vesicle and leakage of inner compounds. DNA was well amplified inside of vesicles, and amplified DNA diffused to the outside was observed using melittin, the most studied antibiotic with the capability to penetrate cell membranes. Confocal microscope was used to observe the entire process. This study shows that vesicles can be used for biomimetic reactors and is expected to lead many advances in synthetic biology and biotechnology.

Poster Presentation : **LIFE.P-189**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

DNA binding and stability study of novel Cu(II) complexes containing quinoline and pyridine

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Biomedical organometallic compounds have been of considerable interest due to their potential applications in biology and medicinal chemistry. Particularly, Cu(II) based complexes have been widely studied as DNA-targeting drugs for medical treatments, which can potentially treat many diseases including cancer, because of their high binding affinity to nucleic acid. Generally, the nucleic acid bound to metal complexes causes increasing their stability. However, very few cases, in which DNA-destabilizing agents have been or are being developed as cancer drugs such as cisplatin, have been reported as having helix-destabilizing properties. In this study, we demonstrate that novel Cu(II) complexes containing quinoline and pyridine cause DNA destabilization. Furthermore, we also explore the binding site of our complexes in DNA in order to determine the reason why destabilized DNA occurs.

Poster Presentation : **LIFE.P-190**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

STING clustering pathway

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Stimulator of interferon genes (STING), transmembrane homodimer located in the endoplasmic reticulum (ER), is crucial for innate immunity. STING is activated by stimuli such as viruses, bacteria, and DNA damage, which induces the production of 2’3’-cGAMP. cGAMP binds to STING and promotes to structural changes and oligomerization. After oligomerization, STING translocates from the ER to Gogi, and three different processes are induced when the translocate STING: type I interferon, inflammation, and autophagy.
In particular, type I interferons are induced as soon as STING exited the ER. However, the signaling pathway of STING in Golgi is unclear.
To investigate Golgi function of STING signaling, we use blue light-induced STING oligomerization system with cytochrome 2 (CRY2) and cytosolic STING. CRY2, a photoreceptor that responds to blue light and then homo-oligolization, was fused with cytosolic STING that is removed transmembrane domain. Under blue light, cytosolic STING was oligomerized but did not translocate to Golgi.
As a result, we confirmed that light induces type I interferon signaling but not inflammation. Our results suggest that STING must translocate to Golgi for inflammation signaling.

Poster Presentation : **LIFE.P-191**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of new technologis to increase the efficiency of insertion-based genome editing

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CRISPR-Cas9 is a next-generation gene-editing technology that has made a significant breakthrough in the treatment of genetic diseases. When the Cas9-induced DNA break is repaired in the presence of donor DNA, the homology-directed repair (HDR) pathway can be exploited to precisely knock in a desired edit at the desired locus. However, a competing repair pathway, non-homologous end joining (NHEJ), is much faster, which can result in unpredictable DNA repair outcomes. HDR-based genome editing is necessary to establish model cell lines and therapeutic cells for various diseases. Therefore, we are developing new technologies to increase HDR efficiency. First, we generate donor DNAs containing Cas9-binding sites, which allows for efficient delivery of the donors into the nucleus along with Cas9. Second, we develop donor DNA constructs that are resistant to nuclease-mediated donor destruction. Finally, we design diverse forms of donors and use a combination of small-molecule drugs to increase HDR efficiency. Overall, our new knock-in platform will be used to generate novel therapeutic modalities.

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Poster Presentation : **LIFE.P-192**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of cell-based therapeutics for diabetes using genome-editing technologies

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Patients with type 1 and late-stage type 2 diabetes ultimately require transplantation of β cells that produce insulin. However, the supply of pancreatic islets is extremely limited since they can only be obtained through organ donation. Thus, methods have been developed to produce stem cell-derived β cells as an indefinite source of insulin-producing cells. However, the use of stem cell-derived β cells is still difficult due to the following issues.1) β cells are highly sensitive to hypoxia and easily lead to apoptosis after transplantation due to the lack of sufficient oxygen supply. 2) β cells are encapsulated into a special device to avoid transplant rejection. However, the device is recognized as an external substance and cause a foreign body reaction, leading to fibrosis around the device and cell death.To solve these problems, we identify several genes that can prevent hypoxia and fibrosis and they are knocked into stem cells using CRISPR/Cas9 technology. The engineered stem cells are then differentiated into β cells, and their performance are verified for use as a cell therapy for diabetes. We will present our recent efforts toward engineering stem cell-derived β cells.

Poster Presentation : **LIFE.P-193**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Targeted Degradation of Steroid Receptor Coactivator-1 through the Hydrophobic Tagging Strategy

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Steroid receptor coactivator-1 (SRC-1) is a transcription coactivator playing a pivotal role in mediating a wide range of signaling pathways by interacting with related transcription factors and nuclear receptors. Aberrantly elevated SRC-1 activity is associated with cancer metastasis and progression, and therefore, suppression of SRC-1 is emerging as a promising therapeutic strategy. In this study, we developed a novel SRC-1 degrader for targeted degradation of cellular SRC-1. This molecule consists of a selective ligand for SRC-1 and a bulky hydrophobic group. Since the hydrophobic moiety on the protein surface could mimic a partially denatured hydrophobic region of a protein, SRC-1 could be recognized as an unfolded protein and experience the chaperone-mediated degradation in the cells through the ubiquitin–proteasome system (UPS). Our results demonstrate that a hydrophobic-tagged chimeric molecule is shown to significantly reduce cellular levels of SRC-1 and suppress cancer cell migration and invasion. Together, these results highlight that our SRC-1 degrader represents a novel class of therapeutic candidates for targeting cancer metastasis. Moreover, we believe that the hydrophobic tagging strategy would be widely applicable to develop peptide-based protein degraders with enhanced cellular activity.

Poster Presentation : **LIFE.P-194**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Effect of Novel Cu complexes on the Fenton-Like Type Oxidative Cleavage of Double-Stranded DNA

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It was well known that reactive oxygen species (ROS) such as superoxide radical (·O2-), singlet oxygen (1O2), and hydroxyl radical (·OH), are essential for human health, disease progression, and therapeutic. Typically, ROS was generated by both endo- and exogenous factors, leading to DNA cleavage through an oxidative pathway or direct cleavage on phosphate, or both. Considering DNA cleavage's benefit, various compounds were developed for potential anticancer drugs. Particularly, transition metal complexes have been investigated extensively due to the diversity of binding mode and their reactivity in DNA. Herein, we introduce the efficient artificial nuclease for mediating DNA cleavage by using novel Cu complexes containing quinoline and pyridine. We also explore the mechanism of DNA Cleavage by our complexes through various scavenger experiments.

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **LIFE.P-195**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

AMPK-induced mitochondrial biogenesis decelerates retinal pigment epithelial cell degeneration under nutrient starvation

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The implications of nutrient starvation due to aging on the degeneration of the retinal pigment epithelium (RPE) is yet to be fully explored. We examined the involvement of AMPK activation in mitochondrial homeostasis and its relationship with the maintenance of a healthy mitochondrial population and epithelial characteristics of RPE cells under nutrient starvation. Nutrient starvation induced mitochondrial senescence, which led to the accumulation of reactive oxygen species (ROS) in RPE cells. As nutrient starvation persisted, RPE cells underwent pathological epithelial-mesenchymal transition (EMT) via the upregulation of TWIST1, a transcription regulator which is activated by ROS-induced NF-κB signaling. Enhanced activation of AMPK with metformin decelerated mitochondrial senescence and EMT progression through mitochondrial biogenesis, primed by activation of PGC1-α. Thus, by facilitating mitochondrial biogenesis, AMPK protects RPE cells from the loss of epithelial integrity due to the accumulation of ROS in senescent mitochondria under nutrient starvation.

Poster Presentation : **LIFE.P-196**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Autophagosome-lysosome fusion is facilitated by plectin-stabilized actin and keratin 8 during macroautophagic process

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Autophagy is a lysosome-mediated degradative process that removes damaged proteins and organelles, during which autophagosome–lysosome fusion is a key step of the autophagic flux. Based on our observation that intermediate cytofilament keratin 8 (KRT8) enhances autophagic clearance in cells under oxidative stress condition, we investigated whether KRT8 supports the cytoplasmic architectural networks to facilitate the vesicular fusion entailing trafficking onto filamentous tracks. We found that KRT8 interacts with actin filaments via the cytolinker, plectin (PLEC) during trafficking of autophagosome. When PLEC was knocked down or KRT8 structure was collapsed by phosphorylation, autophagosome–lysosome fusion was attenuated. Inhibition of actin polymerization resulted in accumulation of autophagosomes owing to a decrease in autophagosome and lysosome fusion. Furthermore, myosin motor protein was found to be responsible for vesicular trafficking along the actin filaments to entail autolysosome formation. Thus, the autophagosome–lysosome fusion is aided by PLEC-stabilized actin filaments as well as intermediate cytofilament KRT8 that supports the structural integrity of actin filaments during macroautophagic process under oxidative stress condition.

Poster Presentation : **LIFE.P-197**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Inhibition of immunoproteasome attenuates NLRP3 inflammasome formation in tumor necrosis factor α-stimulated intestinal epithelial cell

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Excessive release of inflammatory cytokines has been considered as a major cause of chronic inflammation, resulting in intestinal barrier disruption that leads to inflammatory bowel disease (IBD). Tumor necrosis factor α (TNFα) is one of the well-known inflammatory cytokines that activates formation of NLRP3 inflammasome, thus resulting in excessive secretion of inflammatory cytokines causing IBD. Although immunoproteasome inhibitors have been reported to inhibit inflammatory cytokine release, immunoproteasome inhibition has not yet been addressed for attenuation of NLRP3 inflammasome activity in intestinal epithelial cell. Here, we observed that NLRP3 inflammasome assembly was attenuated by peptide epoxyketone YU102, a LMP2 subunit immunoproteasome inhibitor, in intestinal epithelial cell. YU102 also inhibited maturation of active caspase-1 and secretion of IL-1β, which are subsequent inflammatory cascade after the formation of NLRP3 inflammasome. Progression of epithelial-mesenchymal transition and increase of cellular permeability, which were induced by TNFα, were also suppressed through inhibition of immunoproteasome. Furthermore, we found that YU102 does not inhibit degradation of IκBα and its following NF-κB activation that leads to transcription of NLRP3. These findings suggest that inhibition of immunoproteasome with YU102 offers a potential therapeutic premise for prevention of TNFα-induced chronic inflammation through attenuation of NLRP3 inflammasome assembly.

Poster Presentation : **LIFE.P-198**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Selectivity Enhanced Antimicrobial Peptoid by Introducing Novel Cationic Side Chain

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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 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 peptoids demonstrated negligible hemolytic activity with maintaining minimum inhibitory concentration (MIC) values compared to the control. Our study suggests that increasing the cationicity in antimicrobial peptoids can provide a valid strategy to generate a promising antibiotic drug candidate based on peptoid oligomers.

Poster Presentation : **LIFE.P-199**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

H-NS Proteins for Visualization of AT-Specific DNA Sequences

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Various genetic and biological information can be understood by analyzing DNA in a single molecule. Analyzing genetic maps is also important for developing new drugs and medical information. DNA molecules can be observed directly through a fluorescence microscope, and specific information about base sequences can be obtained. In this study, DNA was visualized through a fluorescence microscope by combining DNA binding proteins and fluorescent proteins that bind to specific sequences. As a result, sequence-specific genome maps can be observed, and single-molecular DNA can be visualized with better resolution through both electron microscopy and fluorescence microscopy. This analysis method has the advantage of providing access to DNA sequence information

Poster Presentation : **LIFE.P-200**

Life Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Analyzing Protein-DNA Interaction and DNA Damage Detection Using Oxford Nanopore Sequencing

Yoon Yi Kim

Chemistry, Sogang University, Korea

DNA damage and DNA-bound proteins are biochemically important. DNA damage can interfere with the preservation of genetic information, leading to developmental disorders, cell death, or cancer, while DNA-bound proteins regulate gene expression and epigenetic control. ChIP-seq and related sequencing-based methods for genome-wide mapping of DNA damage and protein–DNA interactions have attracted considerable attention. However, current sequencing-based methods were developed focusing only on positive DNA, which requires time-consuming and large sample preparation. This leads to DNA loss and a longer preparation time. Here, we sequenced the negative DNA to map the DNA damage and protein-DNA interactions using Oxford nanopores. First, detection of SSB (single-strand break) and 8-oxoG (8-oxoguanine) damage is performed by sequencing undamaged DNA (negative DNA) without separation of positive/negative DNA using “nanopore-soni sequencing”. Additionally, protein-DNA interactions can be visualized using "nanopore-block sequencing", which is a novel approach that allows negative DNA sequencing without separation of positive/negative DNA. Nanopore-block sequencing doesn’t need antigen-antibody interaction, it is possible to analyze most proteins if they have an affinity for the DNA molecules. Therefore, this approach has a high potential to replace expensive sequencing-based platforms and small-scale EMSA or FRET for protein–DNA binding analysis. The coverage depth profile of negative DNA sequencing demonstrates the presence of deep valleys, thus providing a map of the DNA damage and protein–DNA interactions. In conclusion, nanopore-soni and nanopore-block sequencing is a simple, inexpensive and promising platform for the studies of the DNA damage and protein–DNA interactions.

Poster Presentation : **LIFE.P-201**
Life Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Bioorthogonal imaging of STING dynamics in live cells

Wonjin Park, **Eunha Kim***

Department of Molecular Science and Technology, Ajou University, Korea

Live cell imaging of the STING protein was achieved using an in cellulo bioorthogonal click reaction with a TCO-fused STING ligand and a tetrazine-fused Near-IR fluorophore. Although TCO conjugation on the STING ligand marginally reduced its binding activity, the TCO-fused STING ligand still exhibited reasonable EC50 and Emax values. Additionally, we observed dose-dependent activation of the STING-TBK-IRF pathway with the compound. Our two-step bioorthogonal approach provided better bioimaging results compared to the one-step approach. We confirmed target specificity via competition assay and imaging experiments with STING knock-out THP-1 cell lines. Interestingly, longer incubation of the TCO-fused STING ligand induced degradation, which was matched by the two-step fluorescent bioorthogonal imaging results. We believe this approach may be beneficial for monitoring STING dynamics in live cells.

Poster Presentation : **ORGN.P-202**

Organic Chemistry

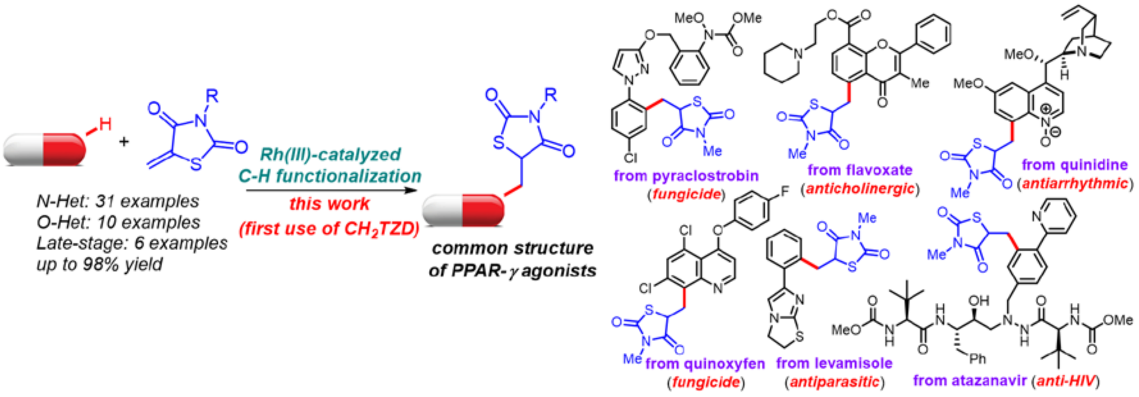
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Innovatory Method for Synthesizing Diabetes Medicine Glitazones: Methylene Thiazolidinediones as Alkylation Reagents via Rh(III) Catalysis

Kyeongwon Moon, Sujin Min, Hyungjin Shin, In Su Kim[*]

School of Pharmacy, Sungkyunkwan University, Korea

The selective modulation of peroxisome proliferatoractivated receptor γ (PPAR-γ) is one of the central topics for the treatment of type 2 diabetes. In particular, a thiazolidine-2,4-dione (TZD) scaffold on glitazones plays a crucial role in selective receptor binding, hence leading to the stimulation of PPAR-γ. A common structural feature of PPAR-γ agonists is the Ar-CH_2-TZD group. The conventional approach for generating this framework relies on the aldol condensation between nucleophilic TZD and aryl aldehydes followed by olefin hydrogenation. However, from the viewpoint of medicinal chemistry and drug development, this strategy presents intrinsic drawbacks, namely, the need for prefunctionalized aldehydes and functional group instability under hydrogenation conditions, which lead to the limited generation of synthetic derivatives. Therefore, the a new methodology for synthesizing the Ar-CH_2-TZD backbone with fewer synthetic steps is in demand. Herein, we first demonstrate the utility of methylene TZD in the C−H functionalization of various (hetero)arenes, affording (Het)Ar-CH_2-TZD. Notably, this protocol provides a valuable opportunity to rapidly access the drug candidates via PPAR-γ modulation. Moreover, the late-stage installation of the CH_2-TZD moiety into complex drug molecules can be an alternative way to afford synergistic and complementary effects of two pharmacological groups in a single molecule.


H
R
O
N
O
S
N-Het: 31 examples
O-Het: 10 examples
Late-stage: 6 examples
up to 98% yield
Rh(III)-catalyzed
C-H functionalization
this work
(first use of CH2TZD)
common structure
of PPAR-γ agonists
MeO
OMe
from pyraclostrobin
(fungicide)
from flavoxate
(anticholinergic)
from quinidine
(antiarrhythmic)
from quinoxyfen
(fungicide)
from levamisole
(antiparasitic)
from atazanavir (anti-HIV)
Me
Cl
F
Ph
OH

Poster Presentation : **ORGN.P-203**

Organic Chemistry

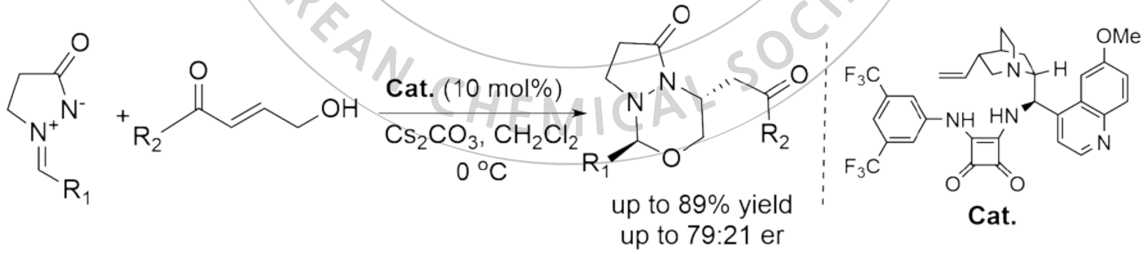
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enantioselective Synthesis of Diazobicyclic Oxadiazines via Organocatalytic [3+3]-Cycloaddition of γ-Hydroxy-α,β-Unsaturated Carbonyls with *N,N´*-Cyclic Azomethine Imines

Sung Hyun Kang, Sung-Gon Kim[1,*]

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

We have developed a highly diastereo- and enantioselective method for synthesizing diazobicyclic oxadiazines through an organocatalytic [3+3]-cycloaddition reaction. Using a squaramide-based catalyst, we were able to carry out the asymmetric cycloaddition of γ-hydroxy-α,β-unsaturated carbonyls with *N,N´*-cyclic azomethine imines to produce enantioenriched diazobicyclic oxadiazines in good yields and with excellent selectivity (up to 10:1 dr and 79:21 er), which are of great interest in biology.



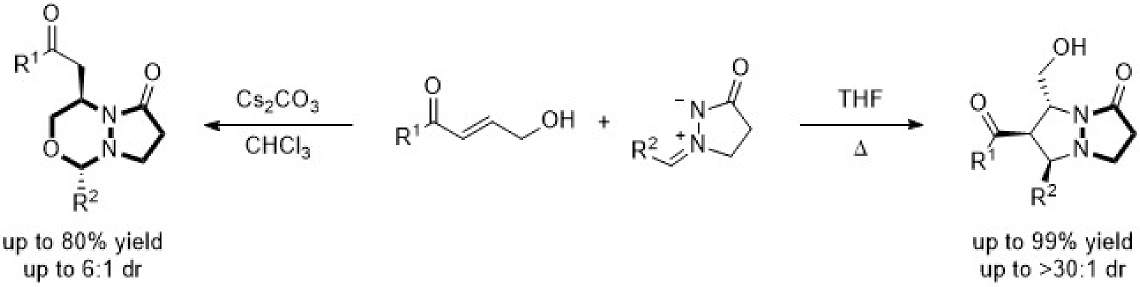
Poster Presentation : **ORGN.P-204**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Chemodivergent 1,3-Dipolar Cycloadditions of *N*,*N*´-Cyclic Azomethine Imines of γ-Hydroxy-α,β-Unsaturated Carbonyls

Sung Hyun Kang, **Sung-Gon Kim**[1,*]

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

The chemodivergent 1,3-dipolar cycloadditions between *N*,*N*´-cyclic azomethine Imines and γ-hydroxy-α,β-unsaturated carbonyls have been successfully established, showcasing the versatility of this reaction. The utilization of Cs_2CO_3 as a catalyst in this reaction led to the formation of highly desirable pyrazoloxadiazinone derivatives through a [3+3] cycloaddition. On the other hand, employing *i*-Pr_2NEt as the catalyst in this reaction resulted in the elegant synthesis of highly sought after bicyclic pyrazolidines in high yields with excellent diastereoselectivities.



Poster Presentation : **ORGN.P-205**

Organic Chemistry

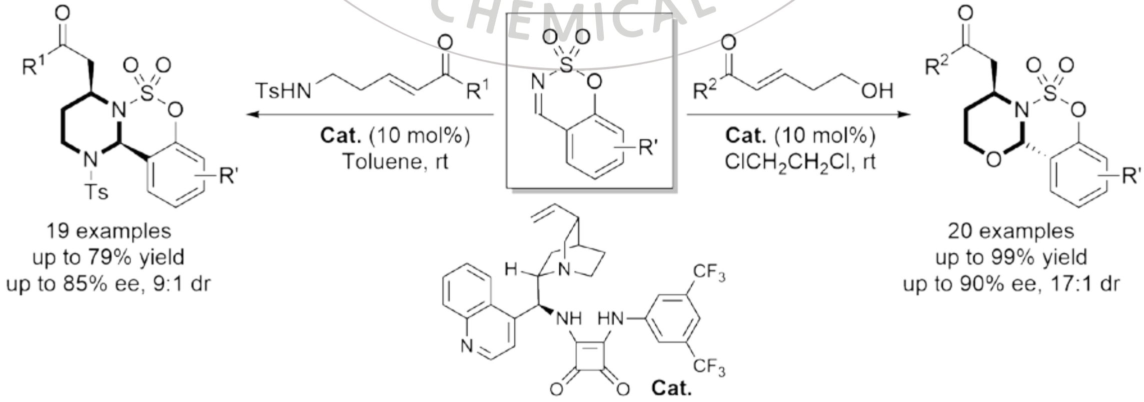
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Organocatalytic enantioselective synthesis of 1,3-oxazinanes and hexahydropyrimidines via [4+2]-annulation of cyclic *N*-sulfimines

Seung Yeon Kim, Sung-Gon Kim[1,*]

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

The asymmetric synthetic method for enantioenriched 1,3-oxazinane and hexahydropyrimidine derivatives via the asymmetric [4+2]-annulation of cyclic N-sulfimines has been established. The reaction of cyclic *N*-sulfimines with δ-hydroxy-α,β-unsaturated ketones afforded a wide range of enantioenriched polyheterotricyclic 1,3-oxazinane derivatives in high yields with good to excellent enantioselectivities in the presence of a cinchonidine-derived squaramide catalyst. This approach has been extended to the asymmetric organocatalytic [4+2]-annulation of cyclic *N*-sulfimines with δ-NHTs-α,β-unsaturated ketones providing enantioenriched hexahydropyrimidines. In addition, the asymmetric [4+2]-annulation of δ-hydroxy- and δ-NHTs-α,β-unsaturated ketones gave their corresponding enantioenriched 1,3-oxazinane and hexahydropyrimidine derivatives with different absolute configurations.



Poster Presentation : **ORGN.P-206**

Organic Chemistry

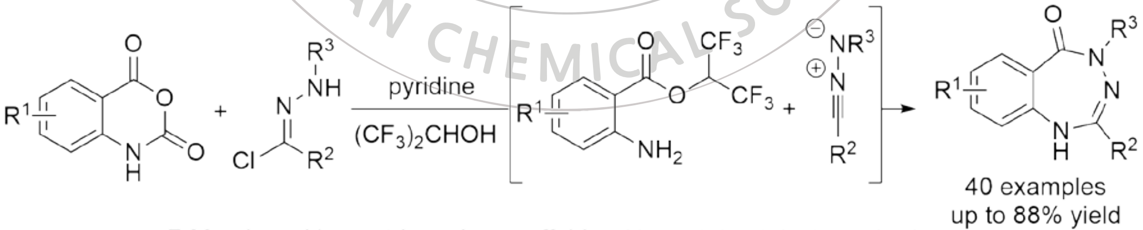
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Hexafluoroisopropanol-Mediated Decarboxylative [4+3]-Annulation of Isatoic Anhydrides with Hydrazonyl Chloride-Derived Nitrile Imines: Access to Benzotriazepinones

ByungJun Park, Han Jiwon[1], Sung-Gon Kim[2,*]

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

A novel and efficient method has been developed for the synthesis of highly functionalized benzotriazepinones via a cascade reaction between isatoic anhydride and hydrazonyl chloride. This reaction involves a substituted [4+3]-annulation of hexafluoroisopropyl 2-aminobenzoates to nitrile imines generated in situ, resulting in the formation of seven-membered benzotriazepinones in moderate to good yields. This approach provides a rapid and convenient route to access structurally diverse benzotriazepinones with a range of functionalities.



- 7-Membered benzotriazepine scaffold
- Broad substrates scope
- No metal-catalyst required
- Functional froup tolerance

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-207**

Organic Chemistry

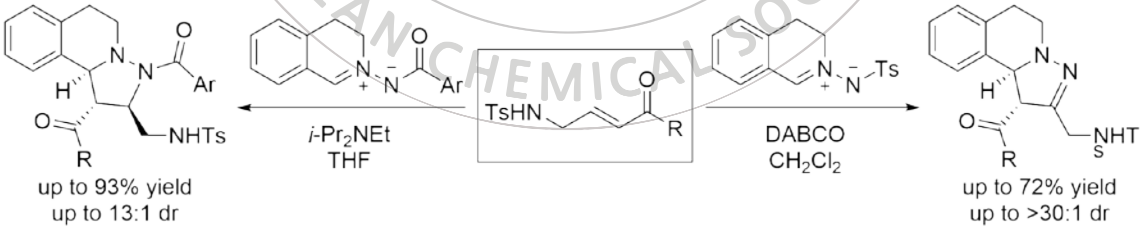
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Chemodivergent 1,3-Dipolar Cycloadditions of *C,N*-Cyclic Azomethine Imines with γ-Sulfonamido-α,β-unsaturated Ketones

Young Jae Yun, Sung-Gon Kim[1,*]

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

1,3-Dipolar cycloadditions of *C,N*-cyclic azomethine imines with γ-NHTs-α,β-unsaturated ketones have been developed to synthesize tricyclic dinitrogen-fused heterocycles. Highly functionalized tricyclic tetrahydroisoquinolines could be readily obtained in good to high yield in the [3+2]-cycloaddition reaction of *N*-Bz-protected *C,N*-cyclic azomethine imines with γ-NHTs-α,β-unsaturated ketones under mild reaction conditions. Moreover, DABCO-catalyzed cycloadditions of *N*-Ts-protected *C,N*-cyclic azomethine imines with γ-NHTs-α,β-unsaturated ketones followed by cleavage of tosyl group is a convenient route to synthesize tetrahydropyrazolo [5,1-a]isoquinolines in good yield with excellent diastereoselectivities.



Poster Presentation : **ORGN.P-208**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

One-pot [2+3]-Cycloaddition/Aromatization of *C,N*-Cyclic Azomethine Imines with α,β-unsaturated Ketones: Facile Synthesis of 5,6-Dihydropyrazolo[5,1-*a*]isoquinolines

Young Jae Yun, Sung-Gon Kim[1,*]

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

An innovative tandem [2+3]-cycloaddition/detosylation/aromatization of *C*,*N*-cyclic azomethine imines with α,β-unsaturated ketones has been developed. This approach involves the base-catalyzed cycloaddition of *N*-Ts-protected *C*,*N*-cyclic azomethine imines with α,β-unsaturated ketones in the presence of DDQ, followed by cleavage of the tosyl group and aromatization. This enables a convenient route for the synthesis of highly functionalized 5,6-Dihydropyrazolo[5,1-*a*]isoquinolines in moderate to good yields.

Poster Presentation : **ORGN.P-209**

Organic Chemistry

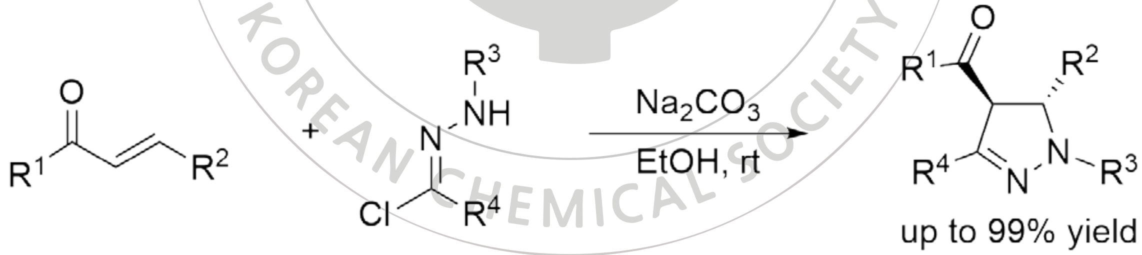
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Stereoselective [2+3]-Cycloaddtion of α,β-Unsaturated Ketones with Hydrazonyl Chloride-Derived Nitrile Imines: Easy access to 4,5-Dihydro-1*H*-pyrazoles

Jiseon Yang, Sung-Gon Kim*

Department of Chemistry, Kyonggi University, Korea

An efficient method for the synthesis of highly functionalized 4,5-dihydro-1*H*-pyrazoles through a [2+3] cycloaddition reaction of various α,β-unsaturated carbonyls with hydrazonyl chloride is presented. The nitrile imines were generated in situ using Na_2CO_3 as a base under EtOH, which provided an attractive strategy for obtaining 4,5-dihydro-1*H*-pyrazoles in good yields (up to 99% yield) and high stereoselectivities (up to 28:1 dr).



up to 99% yield
up to 28:1 dr

Poster Presentation : **ORGN.P-210**

Organic Chemistry

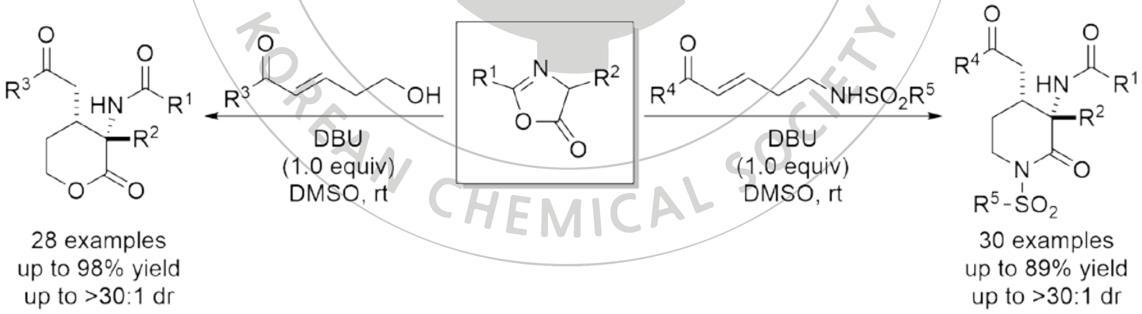
Exhibition Hall 2+3 (1F) THU 11:00~13:00

[4+2]-Annulation of δ-Hydroxy/δ-Sulfonamido-α,β-Unsaturated Ketones with Azlactones for Diastereoselective Synthesis of Highly Substituted 3-Amino-δ-Lactones and 3-Amino-δ-Lactams

<u>Heebum Kim</u>, Sung-Gon Kim[*]

Department of Chemistry, Kyonggi University, Korea

The first base-catalyzed [4+2]-annulation of δ-hydroxy-α,β-unsaturated ketones with azlactones has been developed, through which 3,4-disubstituted 3-amino-δ-lactones were obtained in good yields (up to 98% yield) and with excellent diastereoselectivities (up to >30:1 dr). This approach was extended to the [4+2]-annulation of δ-sulfonamido-α,β-unsaturated ketones, which provided a practical protocol for constructing biologically important 3-amino-δ-lactam frameworks.



28 examples
up to 98% yield
up to >30:1 dr

30 examples
up to 89% yield
up to >30:1 dr

Poster Presentation : **ORGN.P-211**

Organic Chemistry

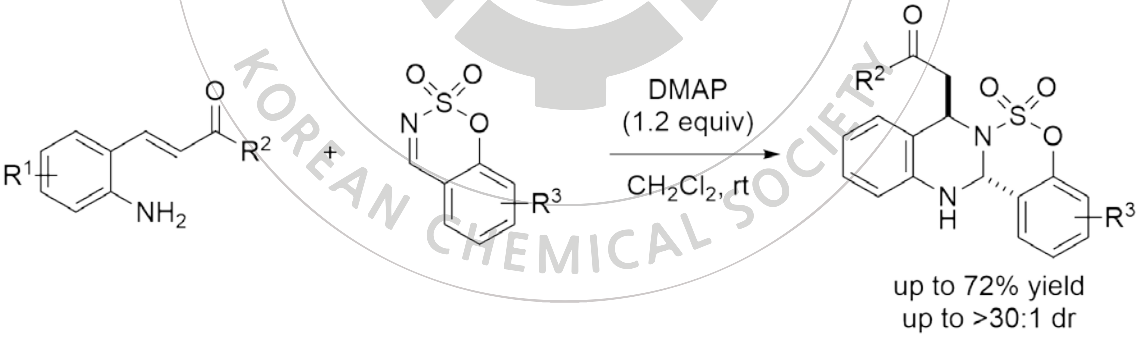
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Stereoselective [4+2]-Annulation of Cyclic *N*-Sulfimines with 2-Aminophenyl α,β-Unsaturated Ketones

Yurim Kim, **Sung-Gon Kim**[*]

Department of Chemistry, Kyonggi University, Korea

We have developed a mild and metal-free synthetic method for the efficient synthesis of tetrahydroquinazoline derivatives via the [4+2]-annulation of cyclic *N*-sulfimines. The reaction involves the use of 2-aminophenyl-α,β-unsaturated ketones and DMAP as a catalyst to afford a diverse range of imidazolidine derivatives with excellent diastereoselectivities and in good yields. Furthermore, we have also established an asymmetric version of the reaction to provide enantioenriched tetrahydroquinazolines.



Poster Presentation : **ORGN.P-212**

Organic Chemistry

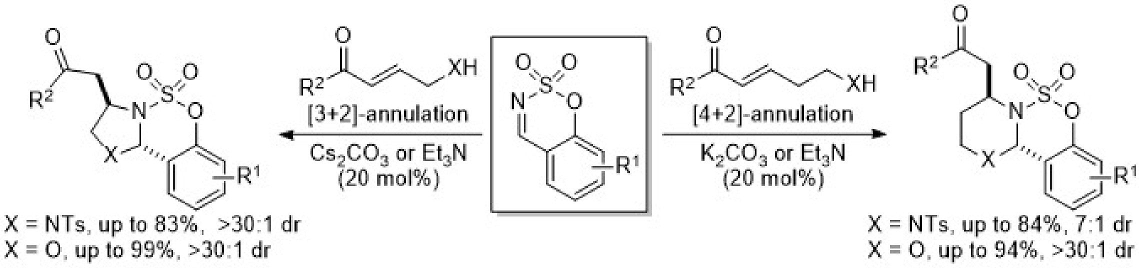
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Base-Catalyzed [3+2]/[4+2]-Annulations of Cyclic *N*-Sulfimines with γ- and δ-Sulfonamido/Hydroxy-α,β-Unsaturated Ketones: Stereoselective Synthesis of Imidazolidines, Oxazolidines, Hexahydropyrimidines, and 1,3-Oxazinanes

Yoseop Kim, Sung-Gon Kim*

Department of Chemistry, Kyonggi University, Korea

A mild and metal-free synthetic method for imidazolidine derivatives via the [3+2]-annulation of cyclic *N*-sulfimines has been established. The reactions of cyclic *N*-sulfimines with γ-sulfonamido-α,β-unsaturated ketones afforded a wide range of imidazolidine derivatives in good yields with excellent diastereoselectivities in the presence of Cs_2CO_3 as a catalyst. This approach extended to the [4+2]-annulation of cyclic *N*-sulfimines with δ-sulfonamido-α,β-unsaturated ketones using Et_3N as a catalyst providing the synthesis of stereoselective hexahydropyrimidines. In addition, synthetic methodologies for the construction of oxazolidines and 1,3-oxazinanes have been established through the base-catalyzed annulation of cyclic *N*-sulfimines with γ-and δ-hydroxy-α,β-unsaturated ketones.



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Poster Presentation : **ORGN.P-213**

Organic Chemistry

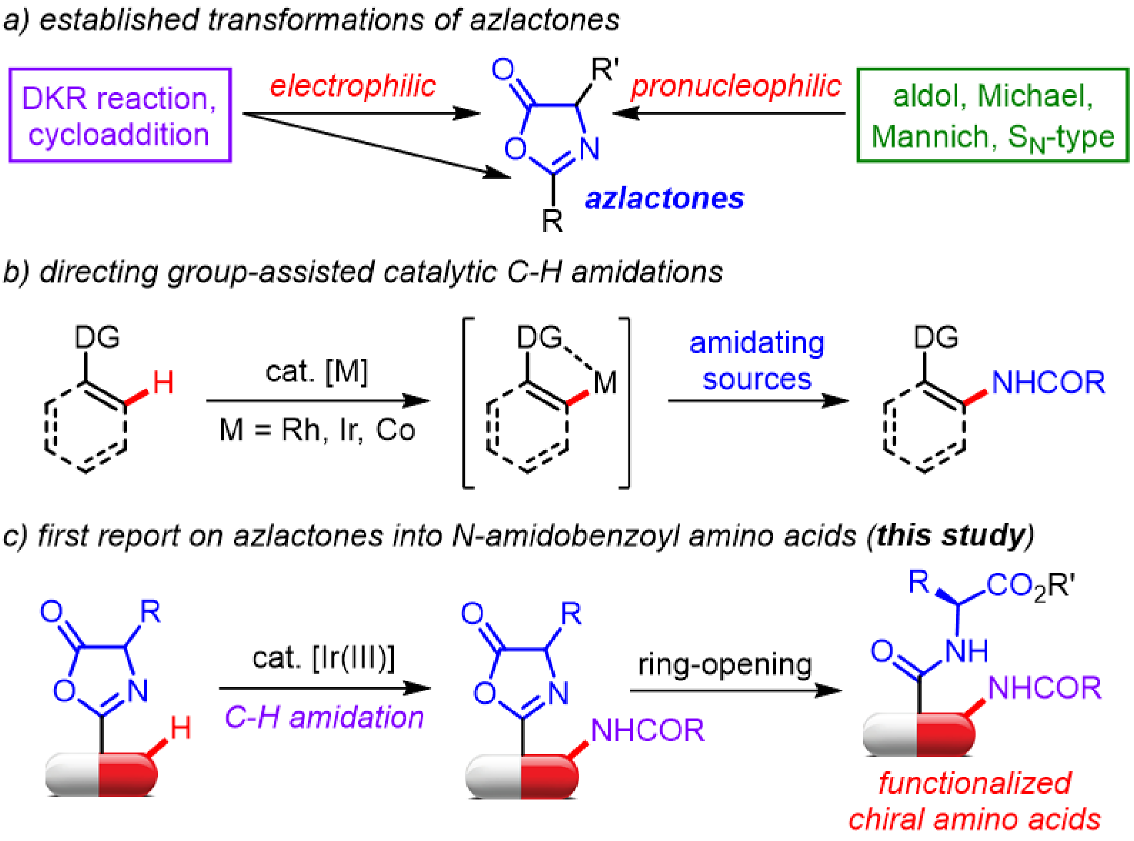
Exhibition Hall 2+3 (1F) THU 11:00~13:00

C–H Amidation of 2-Aryl Azlactones via Ir(III) Catalyst: Application to Chiral *N*-Amidobenzoyl Amino Acids

Eun jae Chung, Heesang Yang, Junhyeok Yang, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

In past decades, the synthesis and modification of amino acid derivatives emerged as important research areas in organic and medicinal chemistry. In particular, functionalized natural and unnatural amino acids proved valuable in drug development, as they often exhibit enhanced bioactivity and pharmacokinetic properties. In this context, azlactones (masked amino acids) have been widely utilized for the synthesis of natural and unnatural amino acid derivatives. Although azlactone cores have been extensively used in C–C bond-forming reactions, the use of azlactone ring as directing group in transition-metal-catalyzed C–H functionalization remains unexplored. In this study, we perform the iridium(III)-catalyzed C–H amidation between 2-aryl azlactones and acyl azides. This transformation reaches to a range of amidated azlactones, which take roles as precursors for chiral amino acids through organocatalyzed ring-opening reactions. To test its effectiveness, we perfrom the azlactone-assisted Ir(III)-catalyzed C–H amidation using acyl azides. Furthermore, we isolate an iridacycle intermediates that supports reaction pathway. In addition, we highlight the this method by the late-stage C–H amidation of drug molecules. Especially, the synthesized adducts are converted into chiral amino acids via urea-catalyzed ring-opening reactions.


a) established transformations of azlactones

b) directing group-assisted catalytic C-H amidations

c) first report on azlactones into N-amidobenzoyl amino acids (**this study**)

Poster Presentation : **ORGN.P-214**

Organic Chemistry

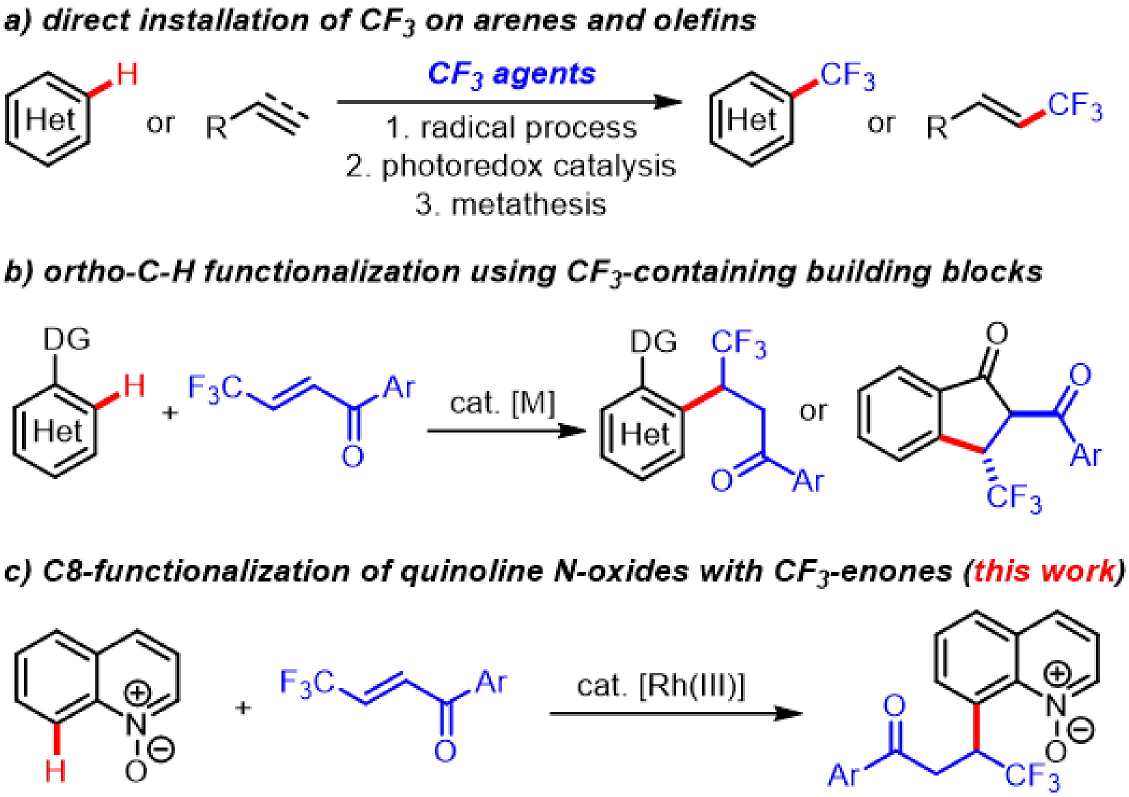
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Quinoline *N*-Oxides through Conjugate Addition with β-CF_3-Enones via Rh(III) Catalyst

Na Young Ko, Jeonghyun Min, Taeeun Kim, In Su Kim[*]

School of Pharmacy, Sungkyunkwan University, Korea

The site-selective incorporation of trifluoromethyl group into biologically active molecules and pharmaceuticals has emerged as a central topic in medicinal chemistry and drug discovery. Tremendous progress has been made on the direct incorporation of a CF_3 group into a series of organic molecules by using trifluoromethylating agents reported by Ruppert-Praksch, Togni, Umemoto, Langlois, and MacMillan (Figure 1a). Recently, β-CF_3-α,β-unsaturated ketones have been also employed in the catalytic C−H functionalizations. For example, Yu and co-workers reported the pyridinyldirected Rh(III)-catalyzed C−H alkylation reaction of aromatic and vinylic C−H bonds with β-CF_3-substituted unsaturated ketones (Figure 1b). Herein, we demonstrate the rhodium(III)-catalyzed conjugate addition of β-trifluoromethylated enones with quinoline *N*-oxides, which result in the generation of β-trifluoromethyl-β'-quinolinated ketones (Figure 1c). The reaction proceeds under mild conditions with complete functional group tolerance. The synthetic applicability was showcased by successful gram-scale experiments and valuable synthetic transformations of coupling products.



a) direct installation of CF_3 on arenes and olefins

b) ortho-C-H functionalization using CF_3-containing building blocks

c) C8-functionalization of quinoline N-oxides with CF_3-enones (this work)

Poster Presentation : **ORGN.P-215**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of the C1-C18 fragment of Neaumycin B

Suin Cho, Duck-Hyung Lee*

Department of Chemistry, Sogang University, Korea

Stereoselective synthesis of the C1–C18 fragment 2 of Neaumycin B (1), 28-membered macrolide compound with 19-chiral centers and 6,6-spiroketal structure, has been described. Brown syn-crotylation and olefin metathesisreaction were used as key steps from (R)-roche ester in the synthesis of C8–C18 fragment 3. C1–C7 fragment 4 was constructed from 1,3-propanediol using diastereoselective allylation, syn-aldol reaction, and olefin metathesis reaction as key steps. Finally, NHK reaction and (S)-CBS reduction as key steps led to the of synthesis of C1–C18 fragment 2 of Neaumycin B (1).

Poster Presentation : **ORGN.P-216**

Organic Chemistry

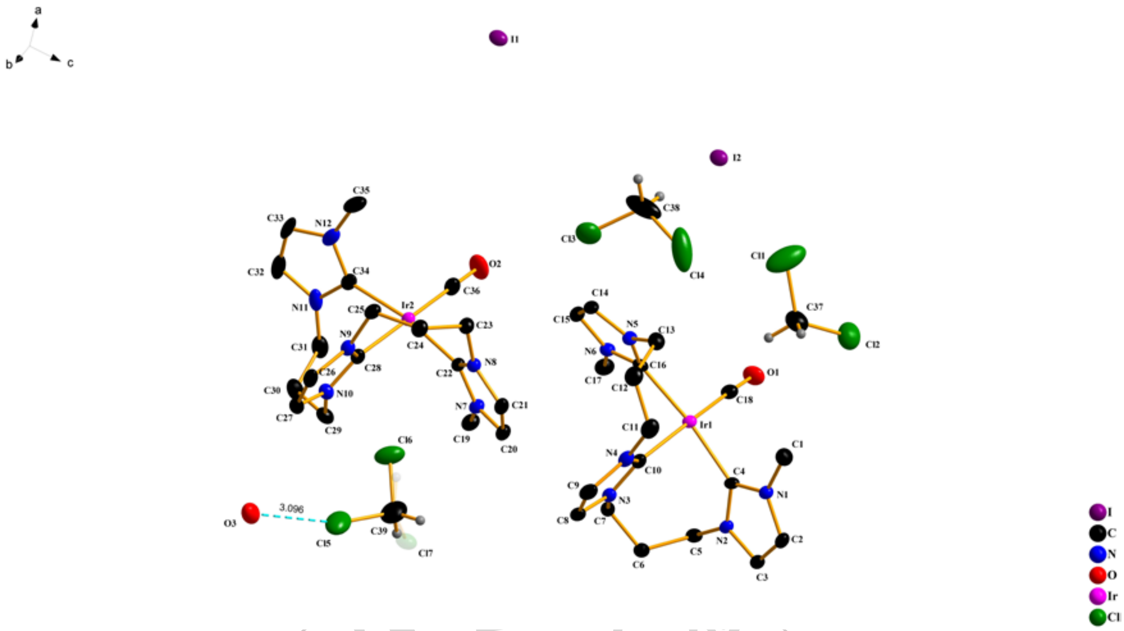
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Comparison Between Ir(NHC) Catalysts in Hydrogen and AHAs Production from Biomass Derivative Ethylene Glycol

Mi-hyun Lee, Heemin Byeon, Hye-Young Jang*

Department of Energy Systems Research, Ajou University, Korea

Ethylene glycol produced from biomass was utilized as a raw material and liquid organic hydrogen carrier in the polymer and chemical industries. Studies on the production of hydrogen from ethylene glycol using transition metal are actively reported. We reported, for the first time, not only the effective production of hydrogen from ethylene glycol but also the synthesis of α-hydroxy acid via homo-coupling of ethylene glycol using newly developed Ir(triNHC) catalysts. We studied the reaction rate and the yield using iridium catalysts possessing different NHC ligands. As a result, we could achieve a high yield and fast rate of hydrogen production through new catalysts synthesized by coordinating three NHCs where strong σ-donating ligands increased the electron density of the metal. Furthermore, we suggest a plausible mechanism of hydrogen production and AHAs synthesis from ethylene glycol utilizing ESI mass analysis and ^{1}H NMR study.


a
b
c
I1
I2
C35
C33
N12
C32
C34
O2
C36
N11
C25
Ir2
C23
C31
N9
C24
C26
C28
C22
N8
C30
N10
C27
C29
N7
C21
C19
C20
Cl6
O3
3.096
Cl5
C39
Cl7
C38
Cl3
Cl4
Cl1
C37
Cl2
C14
C15
N5
C13
N6
C16
C17
C12
O1
C18
C11
Ir1
N4
C10
C1
C4
N1
C9
N3
C8
C7
C5
N2
C2
C6
C3
I
C
N
O
Ir
Cl

Poster Presentation : **ORGN.P-217**

Organic Chemistry

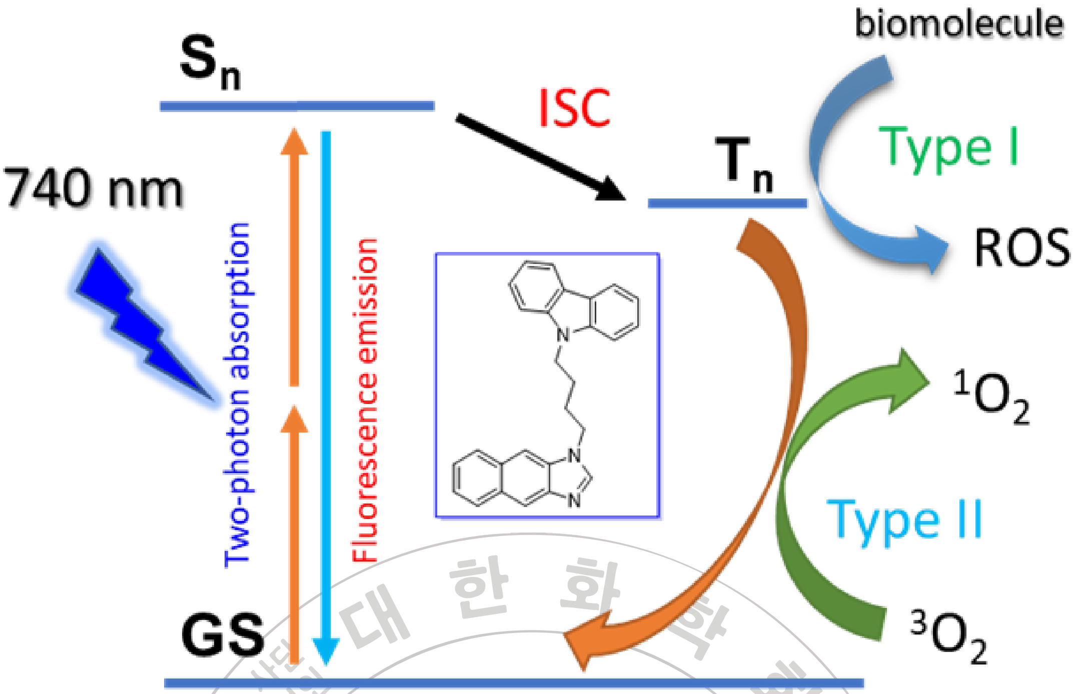
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Heavy-atom-free photosensitizers based Imidazole and carbazole conjugation for two-photon-excited photodynamic therapy and fluorescence bioimaging.

Do Hun Kim, **Songyi Lee**[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Heavy atoms are introduced into photosensitizers (PSs) to enhance intersystem crossing (ISC) processes and Reactive oxygen species (ROS) generation in general. However, the cost and dark toxicity of heavy metals remain big concerns of Photodynamic therapy (PDT) treatment. To overcome the limitations of this, a heavy-atom-free PS was introduced that does not use heavy metals and has high ROS generation efficiency. But loses fluorescence emission ability and makes bioimaging impossible, so it has limitations as a phototheranostic application.Therefore, we synthesized heavy-atom-free PSs BI, CI, and DI suitable as phototheranostic with high ROS generation efficiency and fluorescence emission ability. In the molecular design of BI, CI, DI, the 2 and 3 positions of naphthalene and the 4 and 5 positions of imidazole are conjugated, and the 1 position of imidazole is conjugated with carbazole, 2-bromobenzene, and 2,4-dibromobenzene. In the case of CI, is two photon-excited PDT, It requires long-wavelength light, is relatively harmless to the living body, and has high penetrability. And two photon-excited PDT based on the combination of imidazole and carbazole overcomes the limitations of common two photon-excited PDT and shows high ROS generation and fluorescence emission capabilities.We present a promising framework for designing two-photon-excited heavy-atom-free PSs through a strategy in which the combination of imidazole and carbazole is introduced. In addition, by applying the strategy of introducing the combination of the two moieties, it is expected that it will be of great help in designing phototheranostic materials that can be diagnosed by imaging as well as a cancer treatment.



S_n
ISC
T_n
biomolecule
Type I
ROS
740 nm
Two-photon absorption
Fluorescence emission
N
N
N
$^1O_2$
Type II
$^3O_2$
GS

Poster Presentation : **ORGN.P-218**

Organic Chemistry

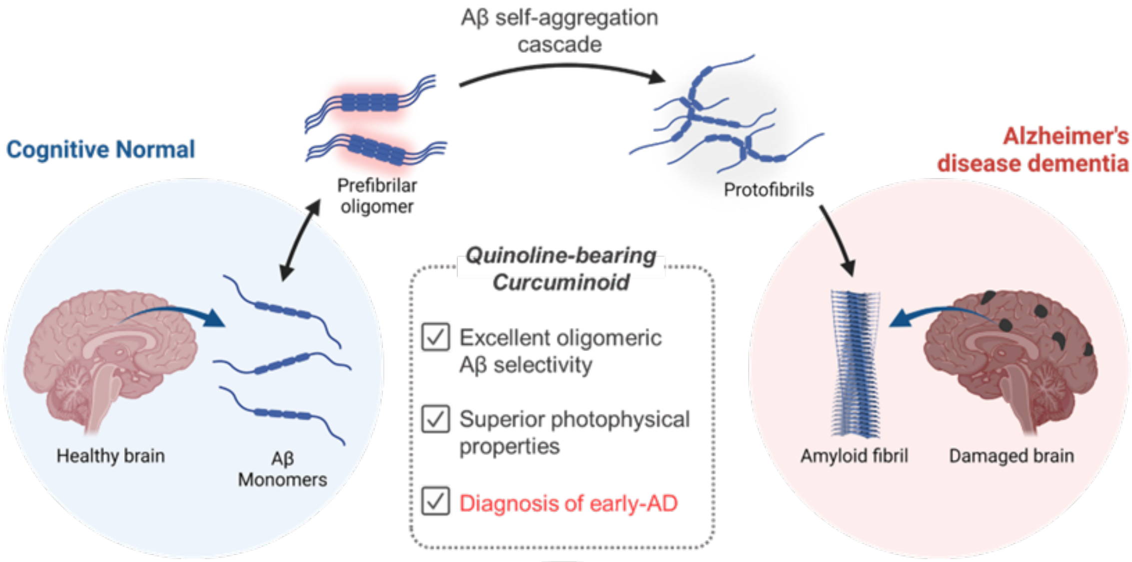
Exhibition Hall 2+3 (1F) THU 11:00~13:00

A small molecule strategy for specific detection of prefibrillar oligomeric Aβ in incipient proteinaceous aggregation cascade

Jusung An, Ji Hyeon Kim, Jaewon Kim, Jungryun Kim, Hyeonji Rha, Jieun Lee, Soyu Zi, Injun Lee, Eun Ji Kim, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Alzheimer's disease (AD), a devastating neurodegenerative disease, affects a large and increasing number of individuals worldwide. According to the amyloid cascade hypothesis, there has been a paradigm shift in understanding the structural basis for these proteinopathies, aqueous soluble oligomeric amyloid beta (*o*Aβ), toxins now widely regarded as instigating neuron damage leading to Alzheimer's dementia. To reveal AD pathology, precise identification and characterization of *o*Aβ in the self-aggregation cascade is significant. However, achievable fluorophores were rarely reported due to the lack of understanding of *o*Aβ's physicochemical properties based on their heterogeneous and transient nature. In the current work, a tremendous small molecule strategy was suggested to rationally design an *o*Aβ-detectable quinoline-dioxaborine-derived probe (**Q-OB**) through finely tailoring amphiphilicity to enhance the binding affinity and selectivity for *o*Aβ via structural modification of biannulate donor motifs in D-π-A dyes. Unprecedented high sensing efficacy was found toward dynamic oligomer monitoring during amyloid fibrillogenesis in vitro and applied to fluorescent detection of the presence of *o*Aβ in cerebrospinal fluid of AD patients. These fluorophores expand the dioxaborine-curcumin-based family of Aβ-sensitive dyes with a promising novel imaging agent. Furthermore, it could be developed preclinical diagnosis platform for the early stages of AD to disrupt pathological progression and build appropriate treatment strategies.


Aβ self-aggregation cascade
Cognitive Normal
Prefibrilar oligomer
Protofibrils
Alzheimer's disease dementia
Quinoline-bearing Curcuminoid
☑ Excellent oligomeric Aβ selectivity
☑ Superior photophysical properties
☑ Diagnosis of early-AD
Healthy brain
Aβ Monomers
Amyloid fibril
Damaged brain

Poster Presentation : **ORGN.P-219**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Palladium and Copper-Catalyzed Fridel Craft Acylation with Activated Amides.

Haeun Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Friedel-Craft type acylation between activated amides and arenes has been realized in the presence of [Pd(cinammyl)Cl]2 and Cu(OTf)2 catalysts. N-Phenyl-N-tosylbenzamide and its derivatives bearing various substituents at the phenyl ring of benzamide reacted with arenes such as mesitylene, toluene, anisole, 4-tertbutylbenzene, o-xylene, m-xylene and p-xylene to produce the corresponding diaryl ketones in moderate and good yields.

Poster Presentation : **ORGN.P-220**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Base-Mediated Synthesis of Anhydrides from Activated Amides

Min Seok Oh, Jonghoon Oh*, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Recently, we reported several transformations of amides into other carbonyl compounds such as primary amides, beta-keto amides, beta-ketoesters, 1,3-diketone, diaryl ketone, acyl fluoride, acyl azide, and urea. In particular, our goal has been the development of a method to synthesize acid anhydride from amide. There is currently only one report of the synthesis of acid anhydride from amide. Szostak and co-workers reported the synthesis of acid anhydrides from twisted amides, using a scandium catalyst. These authors proposed that the nucleophilic addition reactivity was correlated with the amide bond distortion. However, the scope of the substrate was narrow, and moreover, N-benzoylsaccharin exhibited very low activity. Therefore, the development of a more general and simple method for synthesizing acid anhydride from amide is of high interest. Herein, we report a simple and practical method to synthesize acid anhydrides from activated amides in the presence of water (or carboxylic acids) and a base (Scheme 1c). This work represents the continuation of our research on the transformation of amide into other functionalized compounds. Symmetrical anhydrides were synthesized from activated amides such as N-benzoylsaccharins and N-Boc-protected benzamides. The activated amides reacted with H2O in the presence of 1,4-diazabicyclo[2.2.2]octane (DABCO) at 25 °C to produce the corresponding symmetrical anhydrides in high yields through C-N bond cleavage. In addition, N-benzoylsaccharins reacted with benzoic acid derivatives to generate unsymmetrical anhydrides in high yields.

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Poster Presentation : **ORGN.P-221**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Selective Synthesis of Sulfinic and Sulfonic Esters from Sulfonylhydrazides under Electrochemical Conditions

Suji Kim, Jonghoon Oh[1,*], Sunwoo Lee[1,*]

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

Sulfonyl hydrazides have been widely employed as important intermediates using their reactivity releasing hydrazide through S-N bond cleavage. They were used as a sulfonyl source and react with various coupling partners to give the corresponding sulfonylated compounds. Recently, various elegant methodologies have been developed under electrochemical conditions and provided broad substrate scope and mild reaction conditions. During the studies of electrochemical transformations using arylsulfonyl hydrazides, we paid attention to the selective synthesis of sulfonic and sulfinic esters from sulfonyl hydrazide. Hints in the previous reports including ours suggest that choice of counterpart might determine the formation of sulfonic and sulfinic esters. Finally, as this is a reaction using arylsulfonyl hydrazide, it would be expected to proceed under electrochemical conditions and therefore, be complementary to the synthesis of sulfinic and sulfonic esters. Herein, we report selective synthesis of sulfinic and sulfonic esters from sulfonylhydrazides under electrochemical conditions

Poster Presentation : **ORGN.P-222**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nickel-catalyzed directing group assisted reductive coupling of *γ* and *ε* imides with aryl amines a ring opening protocol of Lactams

Karthik rajan Rajamanickam, Sunwoo Lee[1,*]

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

Uncontrolled ring opening polymerization of lactams and hydrolysis of lactams were well known. Ring opening is interesting in Lactams. In this work we have find that in the presence of directing group especially electron withdrawing groups such as benzoyl/sulfonyl groups attached to Nitrogen of a *γ* & *ε*-Lactam selectively gives a ring opened product. Using Nickel as a catalyst. In which we focused on *N*-benzoyl lactams to control the selectivity between ring opened product and transamidated product. In which aromatic amines were reacted with imides in presence of Nickel, Ligand, reductant at 80 oC to get ring opened product no other base and additive required. It showed broad substrate scope and good functional group tolerance.

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Poster Presentation : **ORGN.P-223**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Reductive Cross-Coupling of N-Acyl Pyrrazole and Nitroarene: Synthesis of Secondary Amides

Hayeon Moon, Sunwoo Lee[1,*]

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

Recently, we have developed several amide transformations for the synthesis of another amides, ketones, esters, acyl azides and ketonitriles. During the studies of the amide transformations, we paid attention to acyl pyrazoles as acylating reagents for the synthesis of amides. Acyl pyrrazoles are an important building blocks that are widely used in organic synthesis as intermediates for the preparation of a variety of other organic molecules. They are particularly employed as an acyl synthon in the acyl substitution reactions because they are readily prepared and stable. With these advantages in mind, herein, we report the reaction with acyl pyrazoles and nitro arenes for the synthesis of amides.

Poster Presentation : **ORGN.P-224**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Palladium-Catalyzed Aminocarbonylation: Stereoselective Synthesis of (Z)-β-fluoro-α,β-unsaturated amides

Suhyeon Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Recently, we reported that a variety of 1-fluoro-2,2-diiodovinylarenes were obtained in good yields using the decarboxylative fluorodiiodination of arylpropiolic acid derivatives which can be readily accessible. And we employed them as coupling partners in Suzuki, Hiyama and decarboxylative cross coupling reactions to afford the corresponding mono- and decoupled products. It was found that gem-diiodovinyl compounds have less been studied in the palladium-catalyzed cross coupling reactions. Moreover, they have never been employed as coupling partner in the palladium-catalyzed carbonylations. Based on previous our results, we envisioned that 1-fluoro-2,2-diiodovinyl moiety would be a good source of β-fluoro-α,β-unsaturated building block of amide in the palladium-catalyzed aminocarbonylations. Herein, we report the palladium-catalyzed aminocaronylation of 1-fluoro-2,2-diiodovinylarenes for the selective synthesis of (Z)-β-fluoro-α,β-unsaturated amides.

Poster Presentation : **ORGN.P-225**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Recyclable catalyst of copper nanocluster-bound graphitic carbon nitride for the photo-induced synthesis of arylsulfones

Yubin An, Hyun Min Jung[1,*], Sunwoo Lee[*]

Department of Chemistry, Chonnam National University, Korea

[1]*Department of Applied Chemistry, Kumoh National Institute of Technology, Korea*

A photocatalytic system of Cu(0) nanocluster-bound graphitic carbon nitride (Cu(0)-g-C3N4) was developed for three-component arylsulfonylation reactions. The Cu(0)-g-C3N4 nanocomposite has a structure in which 2–5 nm metallic Cu nanoclusters are anchored on the surface of g-C3N4 nanosheets. The Cu(0) clusters were synthesized by reducing Cu2+ ions with ascorbic acid in the presence of g-C3N4 nanosheets. Cu(0)-g-C3N4 was designed to exhibit dual catalytic activity involving the transfer of photo-induced electrons from g-C3N4 to Cu(0) for the reduction of arylhalides, while the holes in g-C3N4 oxidize the sulfur dioxide anion. The structure of the catalyst was confirmed by electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The well-defined, air-stable Cu(0)-g-C3N4 catalyst effectively promotes the sulfonylation of aryl iodides, thiourea dioxide, and electrophiles to afford the corresponding arylsulfonyl compounds in moderate to good yields. The reusability of the catalyst was also evaluated, and it could be reused up to ten times in arylsulfonylation without the loss of its activity.

Poster Presentation : **ORGN.P-226**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

1,3-Diketone-Mediated Synthesis of Imides from Activated Amides

Miso Kim, Sunwoo Lee[1,*]

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

A variety of methods for the preparation of imides have been reported, ranging from substitution reactions between carboxylic acid derivatives and amides to the oxidation of N-alkyl amides. However, the synthesis of imides via the C–N bond cleavage of amides has not been well developed, even though various transformations of amides have been reported. Therefore, we envisioned that the synthesis of imides via transamidation may provide a very useful tool in the field of organic synthesis. Hence, the 1,3-diketone-mediated synthesis of imides from the reaction between activated amides and LiHMDS is reported herein. Symmetrical aryl imides are synthesized from the reaction of activated amides such as N-phenyl-N-tosyl benzamides. The amine source is provided by lithium hexamethyldisilazide (LiHMDS), and a 1,3-diketone mediates the generation of the N-acyl donor from N,N-bis(trimethylsilyl)amide. Various symmetrical aryl amides are thus formed in moderate to good yields.

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Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Conformational Changes and Stability in Metal-Peptide Networks: A Study of β-Peptide and α/β-Peptide Foldamers

Seoneun Jeong, Hee-Seung Lee*

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

In recent years, metal-peptide networks (MPNs) made of short peptides have gained significant attention due to their structural and functional diversity. This study focuses on using a β-peptide foldamer composed of *trans*-2-aminocyclopentanecarboxylic acid (*trans*-ACPC) as a peptide ligand. The coordination of Ag^+ to the terminal 4-pyridine moieties results in unique metal-peptide networks with different topologies under varying conditions. Distinctive conformational changes are observed in forming metal-coordination bonds from a 12-helix to an 8-helix. On the other hand, using a more flexible α/β-peptide ligand with 2-aminoisobutyric acid (Aib) shows a different behavior. The complexation of α/β-peptide ligands with Ag^+ results in different network structures without the backbone distortion of the α/β-peptides and only 11-helical conformations are observed. The α/β-peptide ligands can be substituted with various α-amino acids with functional groups and still maintain the helical structures of the building blocks, allowing for predictable MPN formation.

Poster Presentation : **ORGN.P-228**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nickel catalyzed conversion of amides to O^{18} labeled-esters

Nithin Pootheri, **Sunwoo Lee**[1,*]

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

O^{18} labelled esters are valuable tools in research and medical applications due to their ability to provide information on the metabolic and biochemical processes within the body. The synthesis of O^{18} labelled esters from readily available primary halides via nickel-catalyzed amide activation in presence of O^{18} water and K_3PO_4 was developed. The reaction is characterized by broad substrate scope and excellent functional group tolerance. The potential of this esterification is highlighted by the late-stage diversification of natural products and pharmaceuticals.

Poster Presentation : **ORGN.P-229**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Unlocking the Structural and Functional Diversity of β-Peptides with Thioamide Modification

Jungwoo Hong, Hee-Seung Lee*

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

Amide Functionality is one of the most important groups in living things and organic chemistry, leading to a growing interest in developing isosteres that mimic their structure and properties. Thioamides, particularly, have received attention due to their structural similarity and hydrogen bonding abilities. However, there is a lack of systematic studies on thioamide-containing peptides, making it hard to display the advantages of thioamide. To address this issue, we designed and synthesized a series of β-peptides decorated with thioamide residues. Interestingly, we discovered an unprecedented, but clear relationship between the thioamide sequence and peptide secondary structure. Furthermore, the introduction of thioamide significantly improved the solubility of the peptides, enabling the synthesis of longer peptides in solution phase with high yields. These findings highlight the potential of thioamides as a promising residue in organic, material, and medicinal chemistry.

Poster Presentation : **ORGN.P-230**

Organic Chemistry

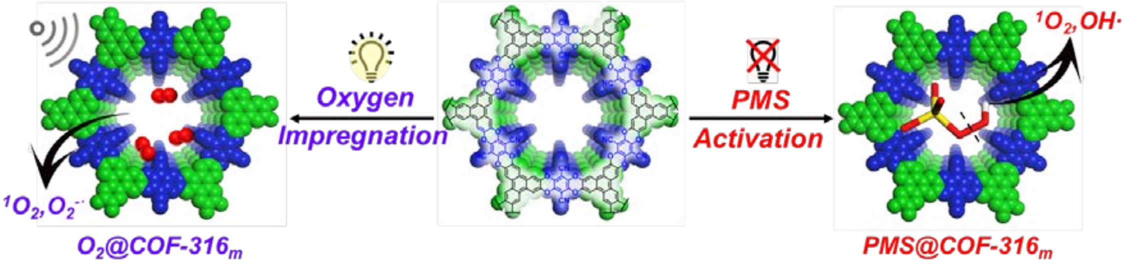
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Photo- and Sonocatalytic ROS generation through a Covalent Organic Framework

Ji Hyeon Kim, Hyeonji Rha, Jusung An, Jungryun Kim, Jaewon Kim, Jieun Lee, Eun Ji Kim[1], Yujin Kim, Soyu Zi, Jong Seung Kim*

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

Reactive oxygen species (ROS) are one of the most useful chemicals in photo-therapeutic and catalytic applications. In order to effectively generate ROS, the role of light-absorbing photosensitizers or activators for pre-ROS sources like peroxymonosulfate (PMS) is significantly essential. Although metal-based ROS generating materials have been widely utilized due to affordable heavy atom effect or viable catalytic sites, the potential toxicity of leached metal ions can be sometimes an undesirable hazard to humans and ecosystems. Herein, we prepared a covalent organic framework (COF) that generates both type I and II ROS upon ultrasound irradiation. In addition, the COF effectively generated ROS through PMS activation even without light sources or cata-lytic metal sites. We also observed synergistic ROS generation by sonosensitization and PMS activation by COF. This work is a demonstration of the COF material functioning as both a sonosensitizer and a PMS activator.



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Poster Presentation : **ORGN.P-231**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Photo-catalyzed double decarboxylative coupling reactions between alkynoic acids and alkyl carboxylic acids

Hyemin Kang, Sunwoo Lee[1,*]

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

Decarboxylative cross coupling reactions have been intensively studied for last decades due to the fact that a variety of organic molecules having a carboxylic acid group are abundant, commercially available, stable and easily handled. It has been reported that aliphatic, aromatic and vinyl carboxylic acids coupled with various counterparts in the presence of transition metal catalyst to give the desired decarboxylative coupling products in good yields. However, the alkylating agent has less employed as a coupling partner in the decarboxylative reaction of alkynyl carboxylic acids. Mai, Sun and co-workers reported copper/silver-catalyzed double decarboxylative coupling reaction of phenylpropiolic acid and aliphatic acids. However, it required high reaction temperature and showed only five examples. Therefore, the development of a more general method of the alkylation for the decarboxylative coupling reaction of alkynyl carboxylic acids is required. Herein, we report the iron-catalyzed double decarboxylative coupling reactions between alkynoic acids and alkyl carboxylic acids under photo reaction conditions.

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Poster Presentation : **ORGN.P-232**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Rational Design of Metal-Peptide Networks with Functional Chiral Channels

Jaewook Kim, Jungwoo Hong, Hee-Seung Lee*

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

Metal-peptide networks (MPNs) are known for their well-defined, chiral porous architectures. This study presents a rational design approach for creating functional chiral channels in MPNs that can host small chiral molecules. Our design involves peptidic foldamers containing α/β-amino acids, which are directional and designable building units due to their rigid conformations. Methionines are incorporated as metal-binding sites to coordinate with Cu clusters, forming crystalline MPNs. A functional residue with a Lewis basic oxygen atom is introduced and positioned near the chiral channel surface, suggesting potential host-guest interactions. The resulting crystal structure of the synthesized MPN reveals chiral channels with a diameter of about 8-10 Å. To evaluate the MPN's ability to separate chiral guest molecules, we soak chiral diols into the crystalline MPN and observe an extended hydrogen bond network between the functional residue and the guest molecule. These findings suggest that our designed MPNs may be well-suited for chiral separation applications.

Poster Presentation : **ORGN.P-233**

Organic Chemistry

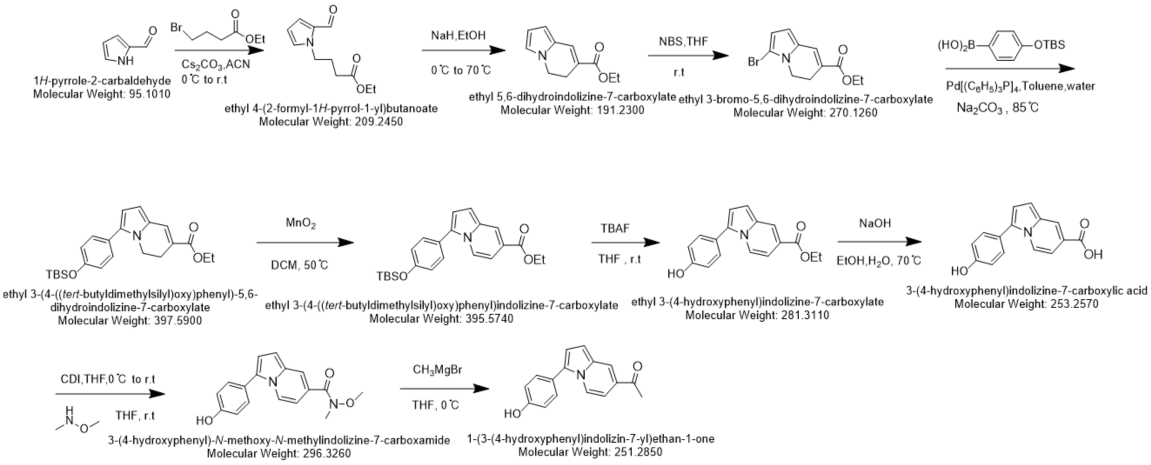
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Modification of fluorescent inolizine and ph Sensor

Min seok Kim[*], **Jonghoon Kim**[1]

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

"In this paper, the structure of indolizine, a type of nitrogen heterocyclic compound, was utilized to synthesize various fluorescent substances. The results showed that indolizine with hydroxyl groups had a long-wavelength fluorescence characteristic. Thus, it was found that it can act as a pH sensor due to the change in the maximum absorption wavelength with respect to pH due to this fluorescence characteristic."



Poster Presentation : **ORGN.P-234**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Molecularly engineered Type-I BODIPY photosensitizers for hypoxia photodynamic therapy (hPDT)

Hyeonji Rha, Ji Hyeon Kim, Jusung An, Jungryun Kim, Jieun Lee, Jaewon Kim, Soyu Zi, Eunji Kim, Injun Lee, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

Photodynamic therapy (PDT), photon-initiated therapeutic strategy that generate cytotoxic reactive oxygen species (ROS), have been interested in fields of cancer eradication. Despite the outstanding advantages of PDT, most of photosensitizers are generally based on oxygen-dependent pathway that generate singlet oxygen via energy transfer (Type-II), which hesitates to harness photo-therapeutic agents for hypoxic solid tumors with insufficient concentration of oxygen. Therefore, type I based photosensitizers that generates superoxide radical, hydroxyl radical, and hydrogen peroxide via electron transfer, have been attracted for overcoming the limitation of conventional photodynamic therapy against solid tumors. Herein, we suggest molecularly engineered type-I BODIPY photosensitizers. As electron donors, thiophene-appended phenylamine groups (such as triphenyleamine, diphenylamine, and carbazole-benzothiophene), are prepared and conjugated with iodinated BODIPY platforms via suzuki couplings to reduce energy gap of intersystem crossing (ISC) process and develop photosensitizers with greater photodynamic performances. Next, we evaluated the photodynamic effects of the photosensitizers (TPA-th-BDP, DP-Bth-BDP, and Cbz-Bth-BDP) with DHR123 (for type I) and DPBF (for type II) assays. Upon the green irradiation, DP-Bth-BDP shows comparable superoxide radical generation, while singlet oxygen is rarely generated. These results demonstrate that photoexcitation of strong donor-conjugated BODIPY PSs leads to electron-transfer mechanism (type-I) rather than energy transfer pathways (type-II), generating oxygen-independent species. Our approach to develop type-I BODIPY photosensitizers provides the appealing solution to hypoxic photodynamic therapy (hPDT).

Poster Presentation : **ORGN.P-235**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

MoO_3 Carbon Nano Tube Catalyst Aerobic Cross-Dehydrogenative-Coupling (CDC) reaction of *N*-aryl tetrahydroisoquinolines with nitro alkanes.

Robin prakash sirvin Rajan, Sunwoo Lee[1,*], Hyun Chul Choi[1,*]

Chemistry, Chonnam National University, Korea

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

An efficient heterogeneous cross-dehydrogenative coupling (CDC) of 2-aryl-1,2,3,4-tetrahydroisoquinolines (THIQs) catalyst by MoO_3 Carbon Nanotube works well without any additive. The novel MoO_3 Carbon Nanotube catalyst system could tolerate various tetrahydroquinoline derivatives and nitroalkanes. The corresponding CDC reaction was obtained in good yields under mild conditions water as green solvent and O_2 as a green oxidant. The reactivity of MoO_3 is enhanced by optimization of different types of CNTs. Also, the catalyst can be easily recovered and reused for the next reaction cycle

Poster Presentation : **ORGN.P-236**

Organic Chemistry

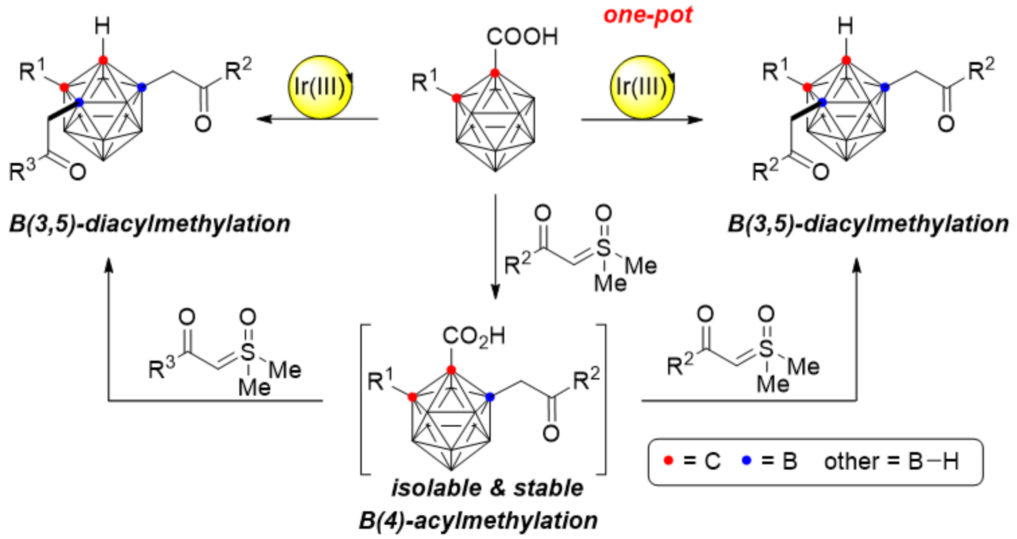
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ir-Catalyzed B(4)-Acylmethylation and B(3,5)-Diacylmethylation from *o*-Carboranes and Sulfoxonium Ylides

Jiwon Kim, Gi Hoon Ko, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Carboranes have demonstrated as functional skeletons in boron neutron capture therapy (BNCT) agents, in building blocks in nanomaterials, and in versatile ligands for transition metals. Generally, because the cage BH proton is less acidic than that of the cage CH proton (pKa ~ 23), cage B−H activation followed by functionalization is difficult compared to that of C−H ones. In addition, since ten BH vertexes are on the carborane, it is much more difficult to control regioselectivity of ten BH vertexes compared to two CH vertexes. Thus, the establishment of efficient method for the introduction of a broad range of functional groups to BH vertexes of carboranes is very fascinating and challenge. Described herein is the first Ir-catalyzed cage B(4)-acylmethylation reaction of *o*-carboranes with sulfoxonium ylides by carboxylic acid-assisted B(4)−H bond activation under extremely mild conditions, producing B(4)-acylmethylated *o*-carboranes and B(3,5)-diacylmethylated *o*-carboranes through sequential B(4)- and B(6)-acylmethylation reaction in one pot.



☑ ***B(4)-acylmethylation***
☑ ***B(3,5)-diacylmethylation***
☑ ***sequential reaction***
☑ ***two-times B−H activation***
☑ ***one-pot procedure***
☑ ***good functional group tolerance***

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Organic Chemistry

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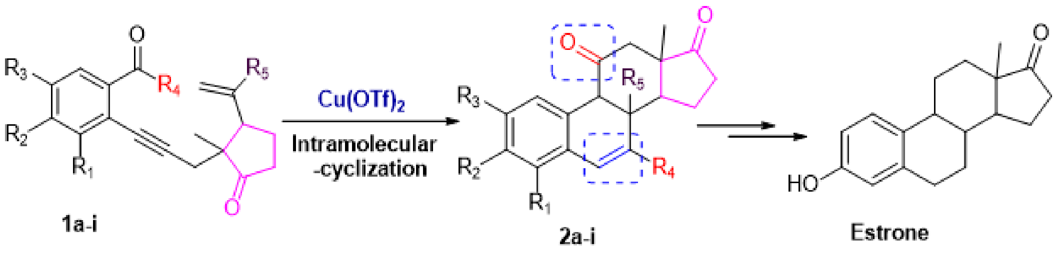
Access toward steroid skeleton and its derivatives via copper-catalyzed intramolecular cyclization: A short synthesis of estradiol and estrone

Liaba Niaz, SooGyum Kim[1,*], Da In Jeong[2,*], Chang Ho Oh[1,*]

chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*
[2]*Hanyang University, Korea*

An effective route of constructing compositions of matter in a cost-effective manner play a significant role towards the synthesis of natural products. In this research, we reported a short methodology towards the synthesis of [6,6,6,5]-tetracyclic compounds as a steroid core through copper-catalyzed cycloaddition of 1,6-enyne-al (1a-i) which were obtained via sonogashira reaction of aromatic substrates with 2-methyl-2-(prop-2-yn-1-yl)-3-vinylcyclopentanone in good yield. In future this methodology will be utilized towards the synthesis of various naturally occurring steroid derivatives.



R_1= H,OCH_3, R_2= OCH_3, H,CH_2-O-CH_2
R_3= OCH_3,H,CH_2-O-CH_2
R_4= CO_2Et,CH_3,H,CO_2CH_3
R_5=H,CH_3

Poster Presentation : **ORGN.P-238**

Organic Chemistry

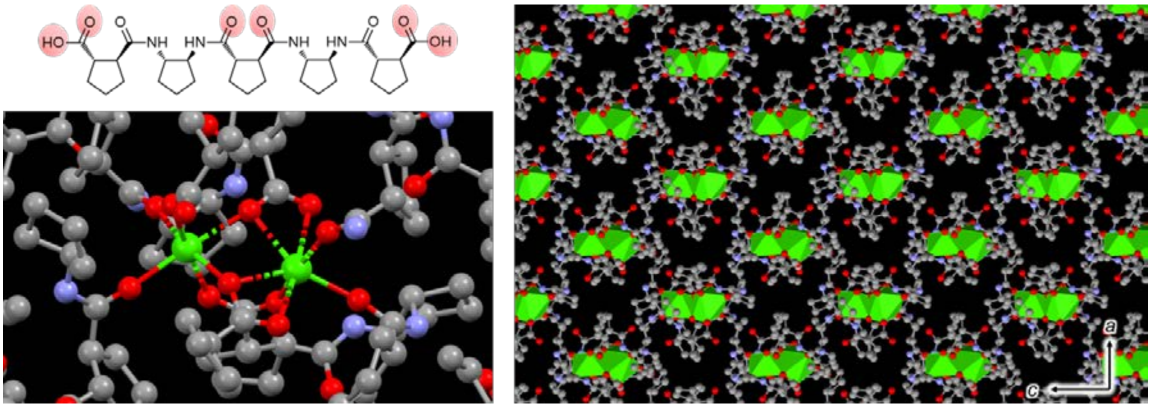
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Designing Metal-Peptide Networks using a CPDADC Foldamer

Youngrok Lee, Jaewook Kim, Hee-Seung Lee*

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

In this study, we aimed to find a more straightforward method for synthesizing metal-peptide networks (MPNs), crystalline structures formed by coordinating metals with peptides as ligands. Although MPNs have the potential for various applications, the synthesis process has been challenging and not as straightforward as metal-organic frameworks (MOFs). To address this issue, we applied the MOF synthesis strategy to MPN synthesis, which typically involves using symmetric linker molecules.We designed a new foldamer called the CPDADC oligomer, which consists of cyclic diamine and diacids and forms C2 symmetric ligands with alternating amide bond directions. Since the CPDADC oligomer is similar to ACPC-based β-peptides, which are known to form stable helix structures, we modified it to coordinate with metals through carboxylate groups at both termini. To demonstrate the effectiveness of this method, we used the CPDADC pentamer and calcium salt to synthesize MPNs. The calcium ions organize high-coordinate clusters and form a robust ionic bond with carboxylate, making it an excellent choice for this synthesis process. The resulting MPNs were highly crystalline, suggesting the potential of this approach for MPN synthesis. With appropriate ligand design, this method can potentially enable the development of new MPNs with unique properties, which could be used in various fields, such as catalysis and materials science.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Poster Presentation : **ORGN.P-239**

Organic Chemistry

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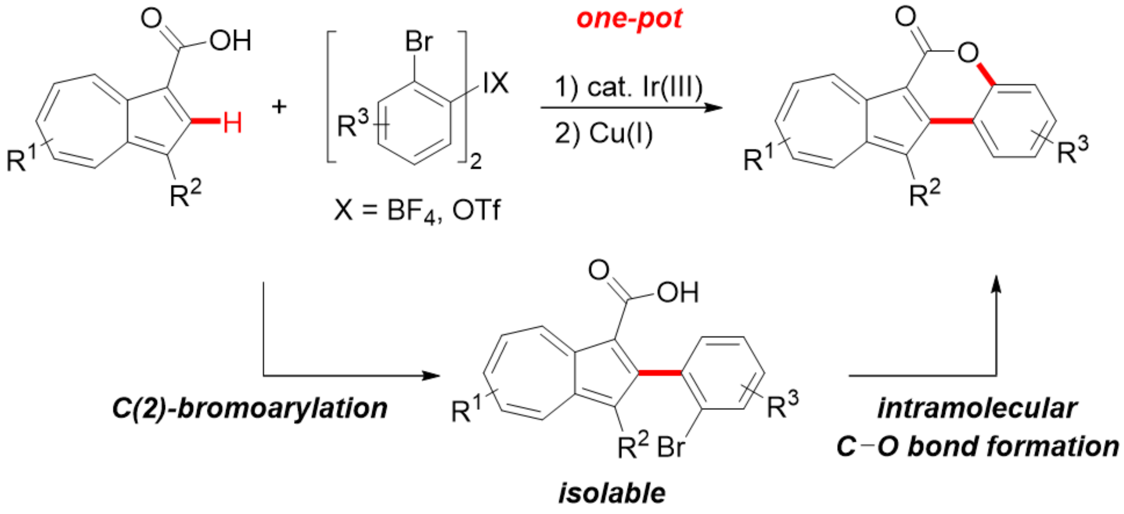
Synthesis of Azulenolactones through Sequential C(2)-Bromoarylation and Intramolecular C−O Bond Formation from Azulene-1-carboxylic Acids with Di(2-bromoaryl)iodonium Salts

Bora Yang, JIwon Kim, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

Azulene, as a representative compound of nonbenzenoid aromatic hydrocarbons, has received much attention due to its importance in natural products, functional materials, and biologically active compounds. Accordingly, the establishment of a streamlined synthetic approach for azulene skeletons from easily obtainable starting materials is extremely important. In particular, as the 2-position of azulene is less nucleophilic than the 1,3-position, the introduction of substituents to the 2-position remains a challenge in organic synthesis. we have demonstrated an iridium(III)-catalyzed C(2)-bromoarylation reaction followed by copper(I)-mediated intramolecular C−O bond formation from azulene-1-carboxylic acids and di(2-bromoaryl)iodonium salts in one pot, resulting in the formation of azulenolactones. The sequential reaction proceeded smoothly via Cu(I)-mediated cyclization of 2-(2-bromoaryl)azulene-1-carboxylic acids derived from the regioselective iridium(III)-catalyzed C(2)-bromoarylation reaction without decarboxylation.



☑ *challenging azulenolactone*

☑ *sequential reaction*

☑ *C–C/C–O bond formation*

☑ *one-pot procedure*

Poster Presentation : **ORGN.P-240**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

3,4-Bis(hydroxymethyl)hexane-1,6-diol-based maltosides (HDMs) for membrane-protein stability

Hyun Sung Lee, Pil Seok Chae[*]

Department of Bionano Engineering, Hanyang University, Korea

Membrane proteins play crucial roles in cellular signaling and communication, making them important targets for biological understanding and drug discovery. For decades, detergents have facilitated membrane protein structural study and thus contributed to advance in our understanding of these important cellular components. However, membrane proteins solubilized in conventional detergents are prone to undergoing aggregation or denaturation over time, particularly for eukaryotic membrane proteins complexes. In an effort to address this issue, we designed and prepared a novel class of detergents, called 3,4-bis(hydroxymethyl)hexane-1,6-diol-based maltosides (HDMs), for use in membrane protein study. We evaluated performance of HDMs compared to two gold standard detergents (DDM and LMNG) using three different membrane proteins, including two GPCRs. This study showed the enhanced stability of the tested membrane proteins solubilized in the HDMs compared to DDM and LMNG. An optimal balance of detergent rigidity and flexibility is likely responsible for the favorable behaviors of the HDMs toward membrane protein stability. Thus, this study not only introduces the new biochemical tools with significant potential for membrane protein structural study, but also suggests a guideline useful for designing novel detergents for membrane protein research.

Poster Presentation : **ORGN.P-241**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Improved pendant-bearing glucose-neopentyl glycols (P-GNGs) for membrane protein study

Taeyeol Youn, Pil Seok Chae[1,*]

Bionano Engineering, Hanyang University, Korea
[1]*Department of Bionano Engineering, Hanyang University, Korea*

Information on membrane protein structures is highly important for biological understanding and drug discovery. Various biomimetic systems have been developed for membrane protein structural study. Detergent micellar system has the ability to extract membrane proteins from the membranes to form protein-detergent complexes (PDCs). Glucoside detergents are particularly interesting as they tend to form small PDCs, a favorable attribute for membrane protein structure determination via X-ray crystallography and cryo-EM. Previously, we introduced pendant-bearing glucoside neopentyl glycols (P-GNGs) that showed enhanced membrane protein stability compared to the original GNG (OGNG). In order to further enhance detergent efficacy for membrane protein stabilization, we prepared more number of P-GNGs by increasing the pendant chain length in this study. Newly prepared P-GNGs contain the main and pendant chains varying their chain lengths from C12 to C15 and C4 to C6, respectively. Most these new P-GNGs gave critical micellar concentrations lower than GNG-3,14, the best P-GNG found in the previous study. This result indicates that the new detergents have the higher tendency to self-assemble in aqueous solution, which could be favorably associated with membrane protein stability. In addition, we found that an increase in the pendant chain length more than C5 substantially decreases the water-solubilities of the new detergents. This result suggests that a pentyl chain (C5) is optimal in pendant size and volume to maximize the hydrophobic effect of detergent molecules without disturbing micellar structure formed by GNG analog with no pendant. We will evaluate these P-GNGs in terms of their effect on membrane protein stability, which provides P-GNGs potentially useful for membrane protein structural study.

Poster Presentation : **ORGN.P-242**

Organic Chemistry

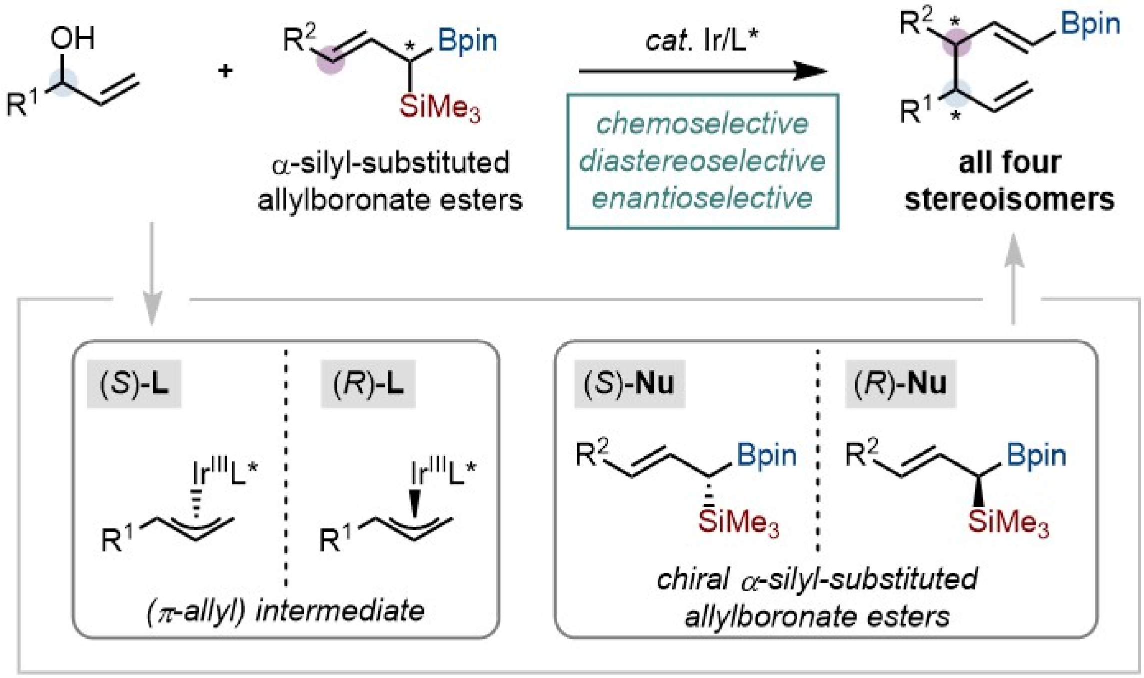
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Iridium-Catalyzed Chemo-, Diastereo-, and Enantioselective Allyl-Allyl Coupling for the Synthesis of (E)-1-Boryl-Substituted 1,5-Dienes with High Stereochemical Control via Chirality Pairing

Yongsuk Jung, Seung Hwan Cho[*]

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

The stereocontrolled synthesis of enantioenriched compounds bearing more than one chiral center is among the most prominent topics in pharmaceutical, medicinal, and organic chemistry. Recent studies have demonstrated that the iridium-catalyzed asymmetric allylic substitution of allyl electrophiles with prochiral nucleophiles is a powerful strategy for preparing enantioenriched molecules with consecutive chiral centers exhibiting high stereoselectivity.Herein, we report a highly chemo-, diastereo-, and enantioselective allyl-allyl coupling between branched allyl alcohols and a-silyl-substituted allylboronate esters, catalyzed by a chiral iridium complex. The a-silyl-substituted allylboronate esters can be chemoselectively coupled with allyl electrophiles, affording a diverse set of enantioenriched (E)-1-boryl-substituted 1,5-dienes in good yields, with excellent stereoselectivity. By permuting the chiral iridium catalysts and the substrates, we efficiently and selectively obtained all four stereoisomers bearing two consecutive chiral centers. Mechanistic studies via density functional theory calculations revealed the origins of the diastereo- and chemoselectivities. Additional synthetic modifications for preparing a variety of enantioenriched compounds containing contiguous chiral centers are also included.


OH
R1
+
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Bpin
SiMe3
*
α-silyl-substituted allylboronate esters
cat. Ir/L*
chemoselective
diastereoselective
enantioselective
R2
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R1
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all four stereoisomers
(S)-L
(R)-L
IrIIIL*
R1
(π-allyl) intermediate
(S)-Nu
(R)-Nu
R2
Bpin
SiMe3
chiral α-silyl-substituted allylboronate esters

Poster Presentation : **ORGN.P-243**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Installation of Free Triazoles and Tetrazoles in Metal-Organic Frameworks

Sangho Lee, Daeyeon Lee, Jooyeon Lee, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-Organic Frameworks (MOFs) are three-dimensional, porous organic-inorganic hybrid materials. MOFs generally have great porosity and low density, therefore, MOFs are considered as a good material for molecular storage, separation, and transportations. Moreover, the chemical and physical properties of MOFs could be controlled by installation of functional group in their pores. The organic functional groups could be incorporated into the ligand part of MOFs. There are two main strategies for functional groups installations of MOFs; pre-functionalization and post-synthetic modification (PSM) by controlling installation step. [1]

Recently, we have successfully installed the coordination-free tetrazoles in Zr-based MOFs. Maximum 50% of coordination-free tetrazoles were incorporated MOFs through pre-synthesized tetrazole-functionalized dicarboxylate ligands. Due to the great acidity of tetrazole, the obtained MOFs were directly applied to proton conduction study.[2] In addition to tetrazole chemistry, the triazole groups have also been successfully incorporated into MOFs. In this case, post-synthetic exchange (PSE) strategy was employed, and the incorporation ratio was controlled by exchange process. The detail procedures for functional group installation along with the preparation of ligands and MOFs will be discussed.

References

1. Kim, D.; Kang, M.; Ha, H.; Hong, C. S.; Kim, M. *Coord. Chem. Rev.* **2021**, *438*, 213892.

2. Lee, D.; Lee, S.; Son, Y.; Kim, J.; Cha, S.; Kwak, D.; Lee, J.; Kwak, J.; Yoon, M.; Kim, M. *Bull. Kor. Chem. Soc.* **2022**, *43*, 912-917.

Poster Presentation : **ORGN.P-244**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Oxidation-Cyclization Cascade Reactions with TEMPO-Functionalized Metal-Organic Frameworks

Daeyeon Lee, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-Organic Frameworks (MOFs) are great platform for catalytic organic reactions due to their coordination chemistry nature and high tunability. Various catalytic species could be installed to either the pore of MOFs and/or the frameworks (i.e., ligand) of MOFs toward heterogeneous catalysis.[1] Not only the heterogeneity, but also the substrate size discrimination could be employed with MOF catalysis. Recently, we have successfully utilized TEMPO radical functionalized MOFs toward organic reactions, especially for aerobic oxidation of aldehydes.[2]

In this presentation, our very recent efforts on TEMPO-functionalized MOFs for the cascade reaction will be discussed. The TEMPO-functionalized MOFs have been successfully applied to cyclization of aminophenol to benzoxazole with aldehydes. The TEMPO-functionalize MOFs could be recycled by simple centrifugation, and showed good functional group tolerances for cyclization. In addition, this cyclization could be performed just after aerobic oxidation of alcohols. The primary alcohols were oxidized to the corresponding aldehydes, and cyclized with aminophenol to the desired benzoxazole derivatives. The detail studies for cascade reactions will be presented with synthetic data.

References

1. Jeoung, S.; Kim, S.; Kim, M.*; Moon, H. R.* *Coord. Chem. Rev.*, **2020**, *420*, 213377.

2. Jong, H.; Hong, S.; Heo, Y.; Kang, H.*; Kim, M.* *Dalton Trans.*, **2021**, *50*, 14081.

Poster Presentation : **ORGN.P-245**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

The lomeguatrib-conjugated temozolomide analog for glioblastoma treatment resistance caused by MGMT

Huiyeon Moon, Ji Hyeon Kim, Jusung An, Hyeonji Rha, Jungryun Kim, Injun Lee, Changyu Yoon, Yujin Kim, Jiyoung Yoo, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Glioblastoma (GBM; grade IV astrocytoma) is the most common and aggressive malignant brain tumor in adults. Median survival from time of diagnosis is only approximately 12 – 15 months. The first-line current standard of care treatment is based on complete surgical resection, followed by concomitant administration of radio-and chemotherapy and adjuvant chemotherapy (Stupp protocol) and standard chemotherapy consists of Temozolomide (TMZ) because it can cross the blood brain-barrier (BBB) and can be taken by mouth. TMZ transfers a methyl group at the N-7 and O-6 positions of guanine and the O-3 position of adenine in the DNA structure. The methylation of the O-6 position of guanine is the most cytotoxic, which leads to cell apoptosis.Although TMZ offers some hope to GBM patients, it is estimated that at least 50% of GBM patients do not respond to TMZ, due to the overexpression of the O^6-methylguanine-DNA methyltransferase (MGMT). MGMT is a DNA repair enzyme that removes the alkyl group in O^6-methylguanine (O^6-MeG). Thus, MGMT inhibitors like lomeguatrib which is a pseudosubstrate for MGMT, are an essential anticancer therapeutic approach to overcome TMZ resistance.Herein, for the treatment of glioblastoma, a small-molecule lomeguatrib-conjugated TMZ analog (TA1) was created that can overcome TMZ resistance and produce therapeutic benefits simultaneously.

Poster Presentation : **ORGN.P-246**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Access to Azetidines via Electrocatalytic Intramolecular Hydroamination of Allylic Sulfonamides

Ahhyeon Choi, Hyunwoo Kim[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

Azetidines are prominent structural scaffolds in bioactive molecules, medicinal chemistry, and ligand design for transition metals. However, state-of-the-art methods cannot be applied to intramolecular hydroamination of allylic amine derivatives despite their underlying potential as one of the most prevalent synthetic precursors to azetidines. Herein, we report 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 directly from allylic sulfonamides. The electrochemical kinetic analysis suggests that the rate-determining step of our protocol is linked to nucleophilic cyclization step including the regeneration of catalyst, which diverges from conventional oxidative metal-hydride hydrogen atom transfer (MHAT) regime under chemical oxidants

Poster Presentation : **ORGN.P-247**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Fluorescence with diverse colors towards abnormal proteinaceous aggragates employing benzimidazole-based ICT fluorophores

Injun Lee, Jusung An, Ji Hyeon Kim, Le Yu, Jaewon Kim, Jungryun Kim, Hyeonji Rha, Jieun Lee, Soyu Zi, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

It is widely accepted that there have been diverse investigations into Alzheimer's disease (AD) which is a serious neurodegenerative disease. Nevertheless, the pathological origin of AD remains a mystery. Abnormal β-amyloid (Aβ) and tau protein deposits are pathological characteristics in AD. In recent years, the emergence of various fluorescent dyes for Aβ is directed at the fact that Aβ has drawn much attention as AD’s main pathological feature rather than tau protein, but tau protein has also gained better importance due to enhancing knowledge of its pathological nature. In this context, multispectral fluorescence imaging (MSFI) makes it possible to distinguish several analytes with just a single fluorophore emitting a fluorescent signal with more than one color. MSFI can recognize different protein aggregates, as fluorescent compounds typically display a different Stokes’ shift (multichromatic response) to various protein aggregates. Herein, we employed and discussed benzimidazole derivatives linked with three types of N, N-dimethyl biannulated groups, BZ1 (benzofuran), BZ2 (quinoline), and BZ3 (naphthalene), exhibiting intramolecular charge transfer (ICT) characteristics in diverse solvents. In addition, a benzimidazole-associated polar sensitivity showed multi-colored behavior. It enabled visualization of the minute differences in micro-environmental polarity between Aβ and tau aggregates, leading to different maximal fluorescent emission wavelengths. BZ2 demonstrated an approximately 30 nm bathochromic shift in maximal fluorescent emission in vitro. As a result, these observations offer the potential for developing a future generation of benzimidazole-derived ICT-based fluorescent probes for identifying and visualizing important analytes in AD research.

Poster Presentation : **ORGN.P-248**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Selective Photosensitizer for ALDH$^+$ Cancer Stem Cells

Jieun Lee, Ji Hyeon Kim, Le Yu, Jusung An, Jungryun Kim, Jaewon Kim, Hyeonji Rha, Eun Ji Kim, Injun Lee, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

Cancer stem cells (CSCs) are a small subpopulation within the tumor site and have self-renewal, metastasis, and drug-resistance properties. Because they survive traditional cancer treatments, targeting CSCs has emerged as a promising strategy to eradicate tumors. Aldehyde dehydrogenase (ALDH), one of the CSCs markers, is an enzyme that converts an aldehyde into carboxylic acid. Here, we have developed a new photodynamic therapy (PDT) agent consisting of an aromatic aldehyde as an ALDH substrate and a photosensitizer substituted with sulfur. We confirmed that the photosensitizer was converted from the aldehyde form to the carboxylic acid form by ALDH and could be well accumulated in CSCs. Furthermore, it could generate reactive oxygen species (ROS) under light irradiation leading to phototherapeutic effects in cancer cells.

Poster Presentation : **ORGN.P-249**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Cascade Diazotization/Intramolecular Radical C–H Heteroarylation Reaction: Synthesis of Tricyclic Tetrazoles

Geon Ryun Park, Chang-Woo Cho[*]

Department of Chemistry, Kyungpook National University, Korea

Tetrazoles are a significant class of synthetic heterocycles with attractive applications in medicinal chemistry. For example, 1,5-disubstituted tetrazoles have been widely incorporated into molecules showing various bioactivities and have been used as bioisosteres of cis-amide bonds in peptides to improve metabolic stability. Among them, tricyclic tetrazoles, such as fused 1,5-disubstituted tetrazoles, have attracted considerable attention due to their importance as key skeletons of potentially bioactive compounds. Here, the cascade diazotization/intramolecular radical C–H heteroarylation of 1-benzyloxy-5-aminotetrazoles and 1-phenethyl-5-aminotetrazoles as substrates using sodium nitrite and acetic acid under mild reaction conditions is presented. The reaction efficiently provided 6*H*-benzo[*d*]tetrazolo[1,5-*b*][1,2]oxazines and 5,6-dihydrotetrazolo[5,1-*a*]isoquinolines as the corresponding tricyclic tetrazole products in good yields. Furthermore, tricyclic tetrazole products bearing bromo substituents were successfully applied to cross-coupling reactions such as Suzuki and Sonogashira reactions.

Poster Presentation : **ORGN.P-250**

Organic Chemistry

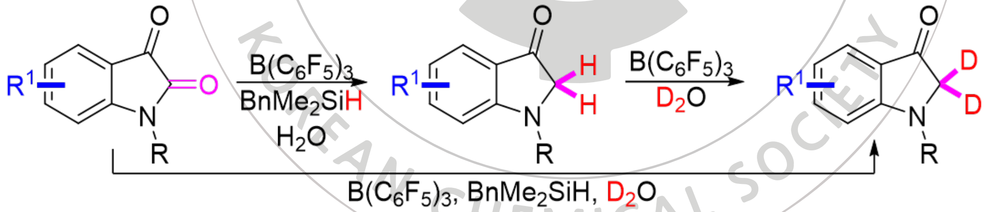
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Modified Chemoselective Reduction and Consecutive Regioselective Deuteration Reaction Catalyzed by $B(C_6F_5)_3$

Hoe Young Choi, Haye Min Ko[1,*]

Department of chemistry, Wonkwang University, Korea
[1]*Department of Applied Chemistry, Kookmin University, Korea*

An efficient chemoselective reduction of isatin derivatives using catalyst $B(C_6F_5)_3$, benzyldimethylsilane, and H_2O is described. Notably, a small amount of water is shown to be a highly effective reaction promoter that decreases the reaction time and temperature for the synthesis of indolin-3-ones. Moreover, using method, excellent deuterium incorporation is achieved *via* the catalytic α-deuteration of indolin-3-ones using $B(C_6F_5)_3$ and D_2O.



- ● ***Short reaction time and mild conditions***
- ● ***Highly chemoselective reaction***
- ● ***C(sp^3)-H Site-selective deuteration***

Poster Presentation : **ORGN.P-251**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Mitochondrial NIR imaging probe mitigating oxidative damage by targeting HDAC6

Jungryun Kim, Le Yu, Jusung An, Ji Hyeon Kim, Hyeonji Rha, Jieun Lee, Injun Lee, Eun Ji Kim, Huiyeon Moon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Despite the apparent abundance of fluorescent probes that target mitochondria, the development of low cytotoxic probes is still required for improved validation of mitochondrial function evaluation. Here, we present T2, a new cyanine-based NIR fluorescent probe that specifically targets mitochondria while posing a remarkably low toxicity risk via modifying intracellular redox status. The newly developed, precisely designed T2 exhibits a significant large Stokes shift, low toxicity, and good mitochondrial retention. Additionally, T2 demonstrated a superior neuroprotection profile in an in vitro model of oxidative stress-induced death by using redox balance to defend against oxidative stress. The current approach, which regulates the redox state at the subcellular level, may offer fresh perspectives on the development of low-toxic fluorescence probes.

Poster Presentation : **ORGN.P-252**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A new small molecule-based dual drug delivery platform for targeting cancer stem cells

Yujin Kim, Ji Hyeon Kim, Jieun Lee, Jusung An, Hyeonji Rha, Soyu Zi, Jungryun Kim, Jiyoung Yoo, Huiyeon Moon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

TNBC is a highly heterogeneous disease, and tumors commonly contain cancer stem cell-like populations with increased self-renewal, tumor invasion, and metastatic abilities. Cancer stem-like cells (CSCs) triggers metastatic recurrence, promotes the emergence of chemoresistance. Then, targeting CSCs can be successful therapy for triple-negative breast cancer (TNBC). We herein present a new small molecule-based dual prodrug conjugated with SN-38 and 3,4-difluorobenzylidene curcumin (CDF), CDF-TM. It can be specifically activated in hypoxic conditions. On in vivo orthotopic allograft model, CDF-TM impairs the dissemination of CSCs from primary allografts and inhibits tumor growth via eradication of CSCs and downregulation of multidrug resistance 1 (MDR1). Also the CDF-TM treatment significantly induces apoptosis in TNBC-derived 3D spheroids, accompanied with caspase-3 activation as well as the attenuation of tumor stemness with evidence of reduction in aldehyde dehydrogenase 1(ALDH1) activity and the CD44high/CD24low phenotype. This novel synchronized dual drug delivery molecule effects on inhibiting tumor growth and metastasis in CSCs, then offers a new therapeutic option for metastatic TNBC.

Poster Presentation : **ORGN.P-253**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Grifolin Synthesis Optimization via competition C-Alkylation vs O-Alkylation

Han Seunghyo, Sangho Koo[1,*]

Department of Chemistry, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Grifolin is a natural compound that can be extracted from mushrooms like Albaterus dispansus. This natural product is used as a treatment because it has the effect of preventing the growth of cancer cells. When we studied grifolin, grifolin was a structure with a farnesyl group attached to orcinol, so we planned to synthesize it using Friedel-craft alkylation, but there are problems of regio-chemistry in orcinol and further cyclization in farnesyl group. So, the plan was changed to use 5-methylcyclohexane-1,3-dione instead of the structure of resorcinol. When reacting a dione with a farnesyl group, studies were conducted on O-alkylation and C-alkylation according to reaction conditions, and detailed results can be found in the poster.

Poster Presentation : **ORGN.P-254**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Systematic Synthesis of Tetraphenyl-Substituted All-E-Carotenoids as Molecular wire

Chibeom Seo, Sangho Koo[1,*]

the chemistry department, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Carotenoids containing phenyl substituents to the polyene chain provide not only improved stability, but also diverse electron-conducting abilities to the chain. We studied the effect of 9,9´,13,13´-tetraphenyl-substituent in the polyene chain of carotenoids as a molecular wires. The synthetic method of tetraphenyl-substituted all-E-carotenes 1 was developed through the formation of tetraphenyl-substituted all-E-apocarotenedial 4, which was prepared by coupling between allylic benzothiazolyl(BT) sulfone 8 and dialdehyde 9. These newly devised building blocks 8 and 9 can be easily synthesized from the common intermediate, 4-chloro-2-phenylbut-2-enal 10. Final olefination of all-E-apocarotenedials and Wittig salt provided all-E-9,9´,13,13´-tetraphenylcarotenes.

Poster Presentation : **ORGN.P-255**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of 1,3- and 1,2-diglycerides of various natural organic acids and phenolic compounds

JiSu Hong, Sangho Koo[1,*]

Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Natural organic acids and phenolic compounds play important roles in physiological activities such as antioxidant, antibacterial, skin damage treatment, skin aging prevention and whitening. These compounds are widely used in cosmetics, pharmaceuticals, and dietary supplements. it is necessary to improve the skin toxicity of natural organic acids and the low skin penetration of natural phenolic compounds. In order to improve those problem, diglycerides of various natural organic acids and phenolic compounds was designed using glycerol. First, 1,3-diglyceride was synthesized by adding epichlorohydrin to a phenolic compound and then combining an organic acids using Bu4NBr catalyst. 1,3-acetal protected glyceral was used to give 2-ester of organic acid in glycerol, deprotection of acetal followed by 2-eterification would give 1,2-diglyceride.

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Poster Presentation : **ORGN.P-256**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Bromoacetate Olefination and Julia−Kocienski Olefination Synthetic Methods for Norbixin and Its Ester Derivative

Aleksei Golikov, Sangho Koo[*]

Department of Chemistry, Myongji University, Korea

Norbixin 1 was efficiently produced by coupling of ethyl bromoacetate with C20 dialdehyde 6 and following double elimination method. Synthesis of norbixin ethyl ester 2 by Julia−Kocienski olefination of novel C7 benzothiazolyl-sulfone 11 and C10 2,7-dimethyl-2,4,6-octatrienedial 12 also were demonstrated. These two concise pathways led to 35% and 36% overall yield of norbixin 1 and norbixin ethyl ester 2, respectively.

Poster Presentation : **ORGN.P-257**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

The synthesis of benzofuran and derivatives by Mn(III)/Co (II) catalysis

Tang Ting, Sangho Koo[1,*]

Organic 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.We found a new way that the furan ring can be smoothly oxidized by MnIII/CoII catalysts,which contributes to the valuable addition to the repertoires of furan oxidation.In the presence of oxygen, 1,4-dicarbonyl moieties was produced by continuous oxidative ring-opening of a furan containing a β-ketoester group at the 2-position via Mn(III)/Co(II) catalyst.Then 1,4-dicarbonyl moieties continuous cyclized with β-ketoester to obtain 4-hydroxy-2-cyclohexanone-1 intermediate.These oxidative cyclization products after continuous aromatization and Paal-knorr reaction, were efficiently converted into multifunctional benzofuran derivatives.

Poster Presentation : **ORGN.P-258**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Application of bimetallic-Mn(III)/Co(II) catalytic oxidative deacetylation of 1,5-dicarbonyl compounds

Hongyu Zhu, Sangho Koo[1,*]

Myungji University, China

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

A method simply contained 4 steps which are Aldol condensation, Michael addition, Mn(III)/Co(II)-catalyzed oxidative deacetylation. Paal-knorr reaction can be applied to the conversion of 1,5-dicarbonyl compounds into 1,4-dicarbonyl compounds, therefore obtaining several various interesting products, such as phenyl-2,2'-bichalcophenes and their aza-analogues, chalcone-derived heteroaromatics, etc. Especially, In this poster, the mentioned compounds will be introduced in detail.

Poster Presentation : **ORGN.P-259**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Phenolic Carotenoids have Superior Antioxidant Activities

Yang Liu, Sangho Koo[1,*]

Myungji University, China

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

We prepared a series of para-phenolic carotenes 1 with ortho- and meta-substitutions and corresponding apo-12´-carotenals 2 by utilizing the benzenesulfonyl protection method. We demonstrated the importance of the ring substituents on their effective conjugation, evaluated by their UV absorption values. 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 2,2´-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) and 1,1-diphenyl-2-picryl-hydrazyl (DPPH) radical scavenging assays.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-260**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Conversion of Ribose and Amino Acids to Pyraline Platform Chemicals and Synthesis of Various Pyrrole-fused Alkaloids.

Huisu Yeo, Sangho Koo[1,*]

Organic chemistry, Myongji univercity, Korea
[1]*Department of Chemistry, Myongji University, Korea*

The one-pot conversion of L-Amino acid and D-Ribose, a reducing sugar, is a method of producing pyrrole-2-carbaldehydes. In order to synthesize substances for pyrrole-based therapeutics that are widely used medically, the pyrraline structure was converted into various polyheterocyclic substances. Five new structures based on pyrrole were designed from the platform pyrrole-2-carbaldehyde. Piperazin-2-one was synthesized using reductive amination with benzylamine. Through further cyclization of ethane-1,2-diamine with the platform, piperazin-2-ones with an imidazolidine ring can be synthesized. In addition, a method for synthesizing piperazin-2-one with oxazolidine through reaction with 2-amino alcohol derived from natural L-alanine, valine, and phenylalanine is proposed. Several series of substances were tested for anti-inflammatory effects by MTT method and Griess assay.

Poster Presentation : **ORGN.P-261**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Photocatalyst-free photoredox reaction of diselenides with aryldiazosulfones: Synthesis of diaryl selenides

RaBin Kim, Dae Young Kim*

Department of Chemistry and Department of ICT Environmental Health System, Soonchunhyang University, Korea

A photcatalyst-free photoredox synthesis of diaryl selenides has been developed by coupling reaction of diselenides with aryldiazo sulfones. The reaction was accelerated under visible light irradiation without using a photocatalyst or photosensitizer. This approach facilitates the synthesis of diaryl selendes with a wide range of functional group tolerance.

Poster Presentation : **ORGN.P-262**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Electrochemical synthesis of bromomethylated γ-lactones via oxidative bromolactonization of unsaturated carboxylic acids

RaBin Kim, Dae Young Kim*

Department of Chemistry and Department of ICT Environmental Health System, Soonchunhyang University, Korea

Electrochemical oxidative bromination and cyclization sequences of unsaturated carboxylic acids were developed in this study. This approach is environmentally-friendly, using bromide anion as bromine radical precursor without external oxidizing reagents. The electrochemical protocol offers a facile way to prepare bromomethylated γ-lactones derivatives in moderate to high yields.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-263**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

One-pot synthesis of 2-amino-4H-chromenes from 2-alkyl phenols via electrochemical oxidation/Michael addition/cyclization sequences

KyeongSeop Kim, Dae Young Kim*

Department of Chemistry and Department of ICT Environmental Health System, Soonchunhyang University, Korea

Electrochemical C-H oxidation/conjugate addition/ cyclization sequences of 2-alkyl phenols with malononitrile are described. This transformation is an environmentally friendly approach by successfully avoiding the use of stoichiometric amounts of external redox reagents. Various 2- amino-4H-chromene derivatives are afforded in moderate to high yields through a one-pot process from 2-benzyl or 2-cinnamyl phenol derivatives under mild reaction conditions.

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Poster Presentation : **ORGN.P-264**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Photocatalytic trifluoromethylation/oxidation/conjugate addition and cyclization sequences of vinyl phenol: Synthesis of trifluoromethylated 4H-1-benzopyran derivatives

KyeongSeop Kim, **Dae Young Kim**[*]

Department of Chemistry and Department of ICT Environmental Health System, Soonchunhyang University, Korea

Visible light-mediated photocatalytic trifluoromethylation, single electron transfer (SET) oxidation, and cycloaddition cascades of 2-vinyl phenols with Umemoto’s reagent and malononitrile were developed. This approach provided the multicomponent synthesis of trifluoromethylated 4H-chromenes via the in situ generation of o-quinone methides, followed by sequential cyclization.

Poster Presentation : **ORGN.P-265**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Organocatalytic enantioselective synthsis of 2-amino-4H-chromenes via C-H oxidation and Michael addition/cyclization sequences

KyeongSeop Kim, Dae Young Kim*

Department of Chemistry and Department of ICT Environmental Health System, Soonchunhyang University, Korea

The chiral 2-amino-4H-chromene derivatives were obtained from 2-alkyl-substituted phenol derivatives in moderate to high yields with excellent enantioselectivities through one-pot cascade via C–H oxidation/Michael addition/ring closure sequences using a binaphthylmodified organocatalyst with low catalyst loading

Poster Presentation : **ORGN.P-266**

Organic Chemistry

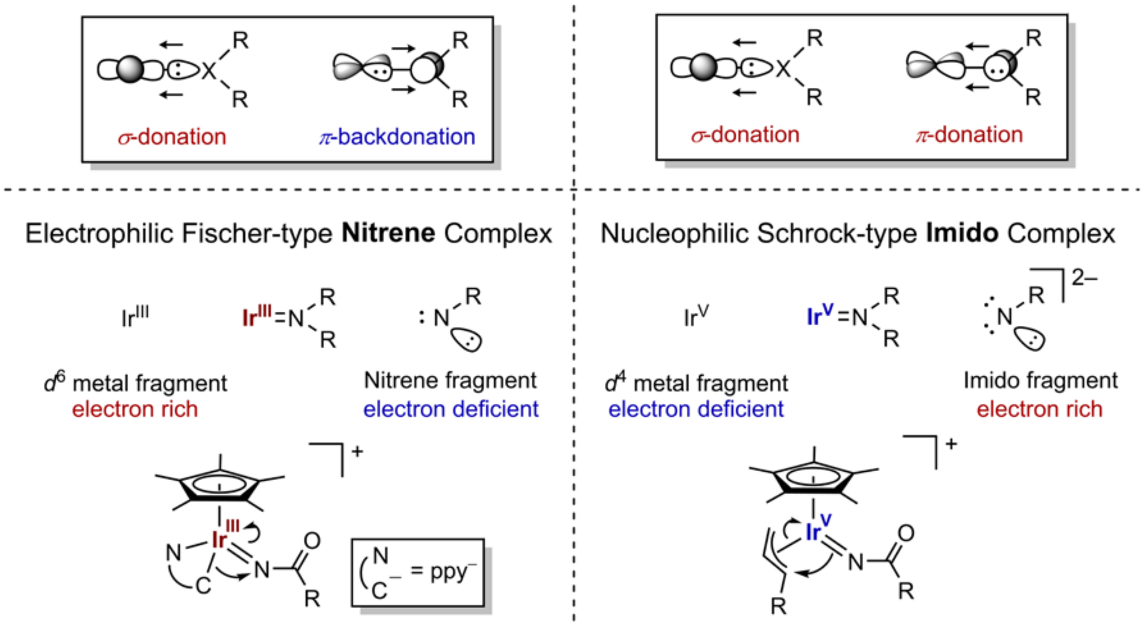
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Revealing an Electronic Structure of the Pianostool Iridium Nitrene

Bohyun Park, **Mu-Hyun Baik***

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

Metal-nitrenes of group IX, such as Ir=NC(O)R or Rh=NC(O)R, are crucial intermediates in C–H amidation reactions using dioxazolone derivatives. Previous studies by Chang and other groups have established the electrophilic nature of these metal-nitrenoids, leading to easy reductive C(sp^3)–N or C(sp^2)–N couplings. However, our recent study, conducted in collaboration with the Blakey group, raised the possibility of the metal-nitrenoid's ability to attack allylic carbon in a nucleophilic manner, challenging the conventional understanding of alkyl or aryl amidations. Herein, we present evidence of the nucleophilic character of iridium-nitrenoid, obtained through both computational and experimental studies. This demonstration broadens the understanding of the behavior of iridium-nitrenes and opens new avenues for their applications in chemical synthesis.



Poster Presentation : **ORGN.P-267**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

An Efficient Method for Ultra-low Branched Polyglycerol Synthesis via Ring-Opening Polymerization of Unprotected Glycidol

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

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

Since the physical properties of polyglycerol can be varied depending on the degree of branching (DB), polyglycerol is promising in the vast polymer industries. Due to the facileness of chain growth at each hydroxyl group of polyglycerol, polymerization of unprotected glycidol with elaborate control of the degree of branching (DB) is rarely achieved. In this study, Cu(triNHC) was successfully employed for the synthesis of polyglycerol with ultra-low degree of branching. This catalytic activity stems from the unique structure of Cu(triNHC) possessing lewis acidic copper center and Brønsted basic carbene. The physical properties of resulting polyglycerols were evaluated by proton diffusion-ordered spectroscopy (DOSY), and gel permeation chromatography (GPC).

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Poster Presentation : **ORGN.P-268**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of NHC-Iridium Catalysts for Generating Sustainable Hydrogen

JaeHo Kim, Mi-hyun Lee, Heemin Byeon, Hye-Young Jang*

Department of Energy Systems Research, Ajou University, Korea

N-Heterocyclic carbene (NHC) ligands have the advantage of forming a stable transition metal by donating electron density, NHCs involving various functional groups can be easily synthesized. Owing to these advantages, research on using NHCs in transition-metal catalysis is being actively conducted. In this study, we are dealing with the Ir(triNHC) catalysts synthetic methods and the structure analysis. We synthesized Ir(triNHC) catalysts by employing NHC ligands as a strong σ donor. Three NHC ligands were coordinated to an Iridium(I) ion, forming stable transition metal complexes. We applied these Ir(triNHC) catalysts to generate hydrogen from biomass-derived alcohol (ethylene glycol). As a result, hydrogen was generated with high efficiency and high speed from ethylene glycol.

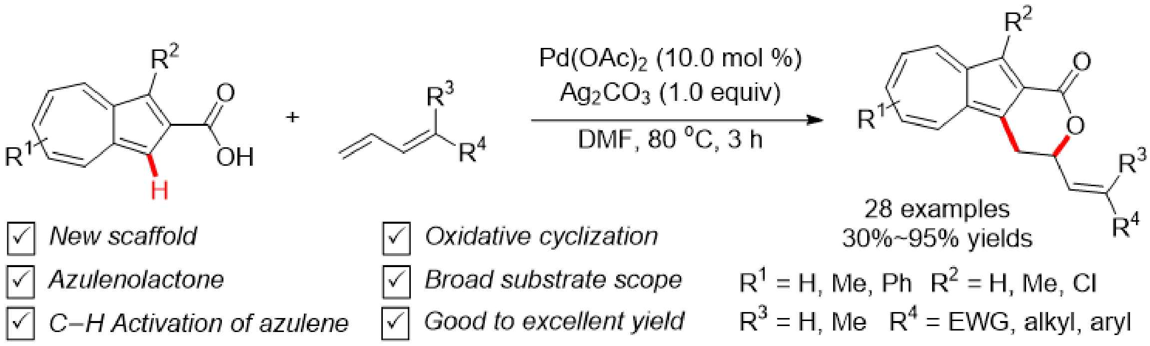
Poster Presentation : **ORGN.P-269**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Palladium(II)-Catalyzed Oxidative Cyclization of Azulene-2-Carboxylic Acids with 1,3-Dienes for the Synthesis of Alkenyl Azulenolactones

Daesu Park, Bora Yang, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

Azulenes, nonbenzenoid aromatic hydrocarbon as constitutional isomer of naphthalene, are finding wide applications in natural products, bioactive compounds, and molecular materials. Thus, the selective introduction of a functional group to azulene skeletone has received much attention. In due course, a variety of methodologies have been demonstrated for the synthesis of a large number of azulene derivatives through transition metal catalyzed selective transformations. Recently, we developed Rh-catalyzed oxidative cyclization reactions of azulene-1- or azulene-2-carboxylic acids with alkynes, producing azulenolactones. However, these methods have the disadvantage that a mixture of azulenolactones is obtained when an unsymmetric alkyne is used. So we envisioned that if 1,3-dienes would be used as coupling partner, then the synthesis of a new skeleton of monosubstituted alkenyl dihydroazulenolactone would be possible through oxidative cyclization. In continuation of recent studies directed toward azulene functionalization and C–H activation, we describe herein Pd-catalyzed oxidative cyclization of azulene-2-carboxylic acids with 1,3-dienes for the synthesis of alkenyl dihydroazulenolactones.



☑ *New scaffold*
☑ *Azulenolactone*
☑ *C–H Activation of azulene*

☑ *Oxidative cyclization*
☑ *Broad substrate scope*
☑ *Good to excellent yield*

28 examples
30%~95% yields

R^1 = H, Me, Ph R^2 = H, Me, Cl
R^3 = H, Me R^4 = EWG, alkyl, aryl

Poster Presentation : **ORGN.P-270**

Organic Chemistry

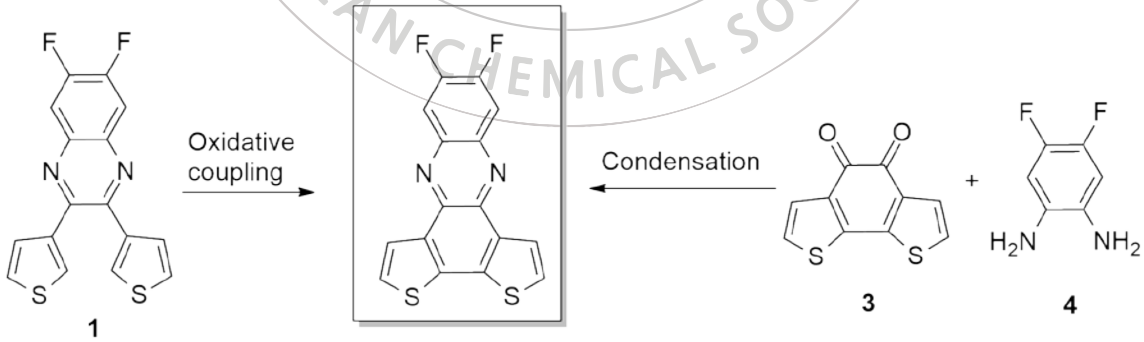
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Highly Efficient Synthesis and Properties of Phenazine-based Monomers for D-A Conjugated Polymers for Organic Solar Cells

Kyukwan Zong*, Hwanhee Jo

Department of Chemistry Education, Jeonbuk National University, Korea

Recently the donor polymers consisted of quinoxaline unit have been known that some of the solar cells fabricated from them showed excellent PCEs.1 The structure of quinoxaline is similar as that of phenazine in terms of containing pyrazine unit. We hypothesized that optical properties of the monomer containing phenazine was similar as those of quinoxaline unit. In this study we have developed new routes for phenazine-based donor units in order to apply for organic solar cells. As shown the following scheme, one of them is rendered from the conversion 1 into 2 by oxidative aromatic coupling reaction. The other is accomplished through condensation of diketone 3 and diamine 4 in final step. In this presentation, synthetic details, scopes and limitations of two synthetic approaches will be discussed. References1.Sun, C.; Zhu, C.; Meng, L.; Li, Y. Adv. Mater. 2021, 2104161.



Phenazine Derivative
2

Poster Presentation : **ORGN.P-271**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Sustainable Production of Formate and Lactate through Iridium-Catalyzed Transfer Hydrogenation of Glycerol Carbonate

Heemin Byeon, Mi-hyun Lee, Hye-Young Jang*

Department of Energy Systems Research, Ajou University, Korea

Studies on transition metal-catalyzed transfer hydrogenation of carbonate have been actively reported. However, they should require high pressure of H2 gas or additional hydride sources. In this study, we reported the first example of Iridium(NHC)-catalyzed intramolecular transfer hydrogenation using glycerol carbonate. The described reaction provides a sustainable route to produce industrially-valuable formate and lactate with high TONs. The reaction mechanism is probed based on control experiments, and the origin of the high catalytic activity of bimetallic Ir(triNHC) was speculated based on the proposed reaction mechanism.

Poster Presentation : **ORGN.P-272**

Organic Chemistry

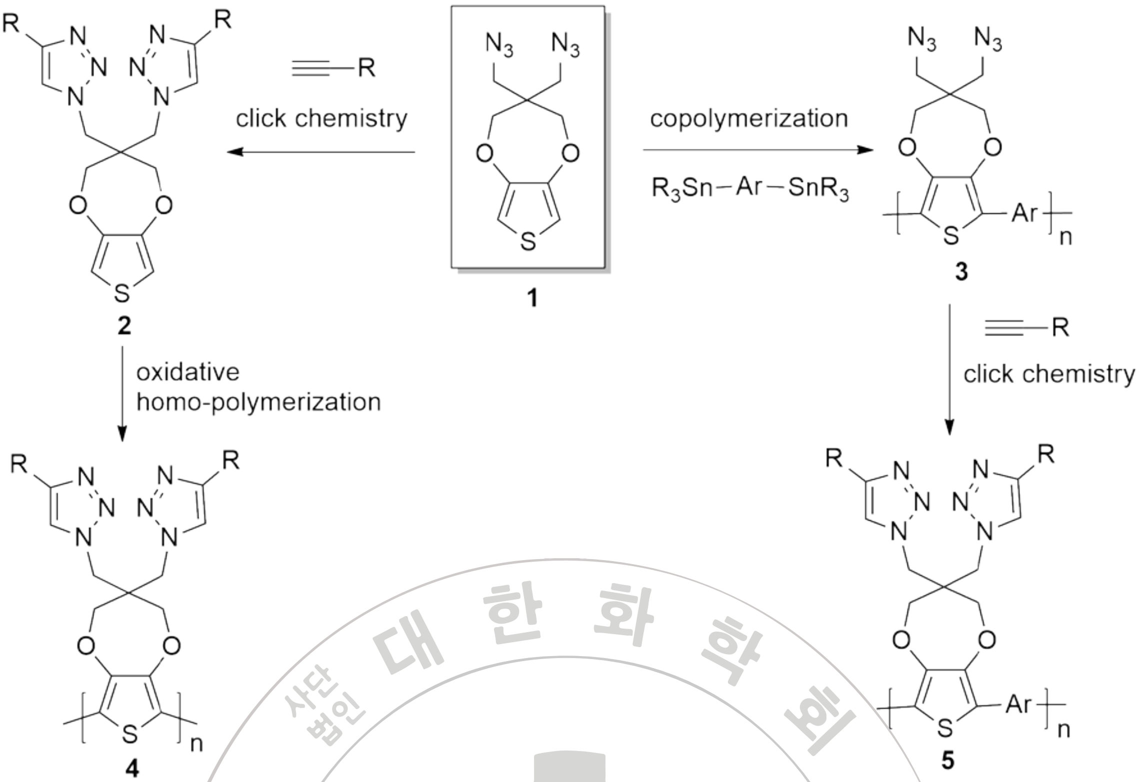
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Characterization of 3,3-Bis(azidomethyl)-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepine (ProDOT-AM2) and Its Derivatives Appending with 1,2,3-Triazole Moieties by Click Chemistry

Kyukwan Zong*, JunMo Kang

Department of Chemistry Education, Jeonbuk National University, Korea

ProDOT (3,4-propylenedioxythiophene) and their derivatives have widely used as the monomers of conducting polymers in the field of OFETs, OPVs, LEDs, supercapacitors, and electrochromic materials.1 With rapid expansion of the field of organic electronic materials, new derivatives of ProDOT have been needed for growing area of organic electronics. In the course of continuing our work to develop new ProDOT derivatives, we have focused on the building block compounds that can be easily derivatized into a variety of useful derivatives simply by click-chemistry. As illustrated in the figure, we found that azide functionalized monomer 1 is a useful monomer which can be easily converted into a wide variety of monomers by a simple click chemistry and also can be used for copolymerization as various donor moieties. Spectroscopic and optical data of the compounds will also be discussed. References1.Handbook of Conducting Polymers, 3rd ed.; Skotheim, T. A., Reynolds, J. R., Eds.; CRC Press: Boca Raton, FL, 2007.


1
2
3
4
5
click chemistry
copolymerization
$R_3Sn-Ar-SnR_3$
oxidative homo-polymerization
click chemistry

Poster Presentation : **ORGN.P-273**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Copper-Catalyzed Radical C−C Cross Couplings of Tertiary Alkyl Halides

Serim Choi, YongSeok Choi[1], Sarah Yunmi Lee[*]

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

We report here the copper-catalyzed carbon-carbon bond-forming coupling reactions of tertiary alkyl bromides with secondary arylamines enabled by bidentate nitrogen-based ligands. The key to achieve this reactivity was to design and synthesis of new ligands. Our coupling reaction proceeds under mild conditions without the aid of external oxidants or light. Various arylamines can be efficiently coupled with an array of tertiary alkyl bromides to furnish lactams containing a quaternary carbon center in good yields. Mechanistic studies including reactivity as well as spectroscopic investigations revealed that this reaction involves a radical intermediate.

Poster Presentation : **ORGN.P-274**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Design and synthesis of novel tabamide A analogs

Jungwoo Hong

Hallym University, Korea

Phenol compounds, which are one of the most abundant secondary metabolites in plants, have various biological activities in addition to having food and nutritional properties. Among the phenolic compounds, phenolic amides are only a small number, but they are known to have interesting medicinal effects such as anticancer and antiviral. Tabamid A, the phenolic amides extracted from *Nicotiana tabacum*, showed the best tobacco mosaic antiviral effect. In this study, compounds that can improve physiological activity through structural modification of tabamide A were designed and synthesized.

Poster Presentation : **ORGN.P-275**

Organic Chemistry

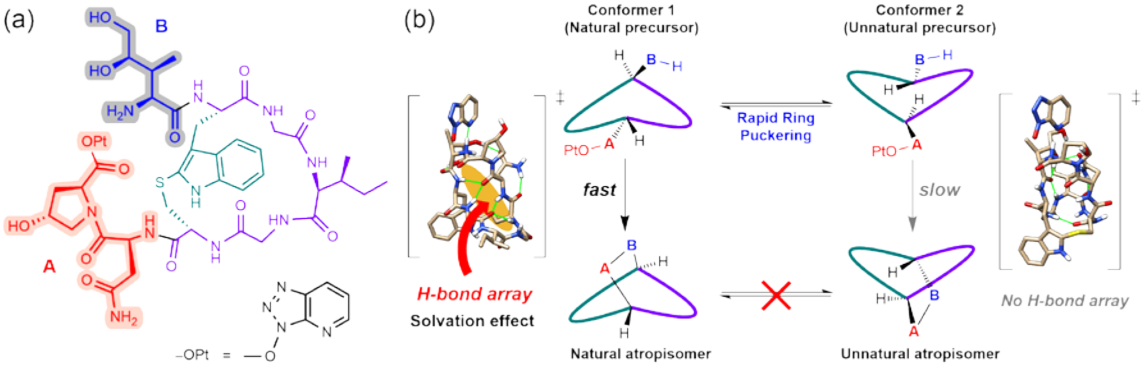
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Understanding Amanitin Atropisomerism

Chattawat Thangsrikeattigun, Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Atropisomers are stereoisomers existing due to high energy barriers for interconversion caused by factors such as steric strain. One example is α-amanitin, a bicyclic octapeptide composed of a macrolactam and a tryptathionine cross-link, preventing bridge flip. α-Amanitin is one of the deadliest of all the toxins found in various species of the mushroom genus Amanita. In 2021, Süssmuth and co-workers reported an efficient and atroposelective total synthesis of α-amanitin. However, the question of what influences the occurrence of the major atropisomer remains, given that the intermediate cyclic polypeptide can be highly flexible. To address this, multi-scaled calculations were performed to investigate the crucial steps of the bicyclic construction. Metadynamics MD simulation unambiguously confirmed that the conformation of the cyclic precursor is scrambled as the ring puckering barrier is small. DFT results indicated that the origin of the atroposelectivity was primarily due to the difference in solvation stabilization between natural and unnatural transition states of macrolactamization. The transition state in the natural conformer shows a significant solvation stabilization due to the formation of four hydrogen bonds in the main chain, resulting in the highly negatively charged region resembling DNA major groove.



Poster Presentation : **ORGN.P-276**

Organic Chemistry

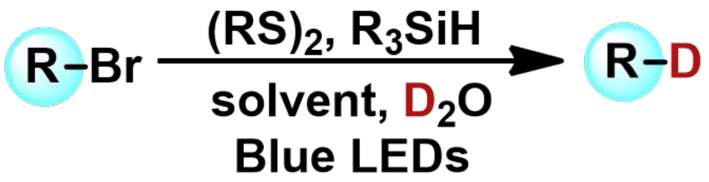
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Radical deuteration of alkyl bromides using disulfide and D_2O under blue light irradiation.

Lee Jiin, Sunggi Lee[*]

Dept. of Physics and Chemsitry, Daegu Gyeongbuk Institute of Science & Technology, Korea

The greatest interest in developing the deuteration of drugs or drug candidates has exploded to improve their metabolic and pharmacokinetic properties. A variety of methods for the deuteration of organic molecules have been developed. Among them, dehalogenative deuteration has been identified as direct tool for delivering deuterium at the target molecule. However, the reported success has employed expensive catalysts or is limited to alkyl iodide. Developing a practical and environmentally benign protocol is still challenging. Herein we report a mild and practical method for the deuteration of alkyl bromides using halogen-atom transfer (XAT) mediated by silyl radical, initiated by thiyl radical generated from homolytic cleavage of disulfide, under blue light irradiation. Furthermore, deuterium oxide (D_2O) was employed as an economical deuterium source. In our system, deuterated products are generated in high yield and excellent D-incorporation at room temperature. Moreover, various pharmaceutical derivatives are well tolerated under these conditions.



- **Mild reaction condition**
- **Simple and practical procedure**
- **Commercially available reagents and D-source**
- **Economic and eco-friendly reaction**

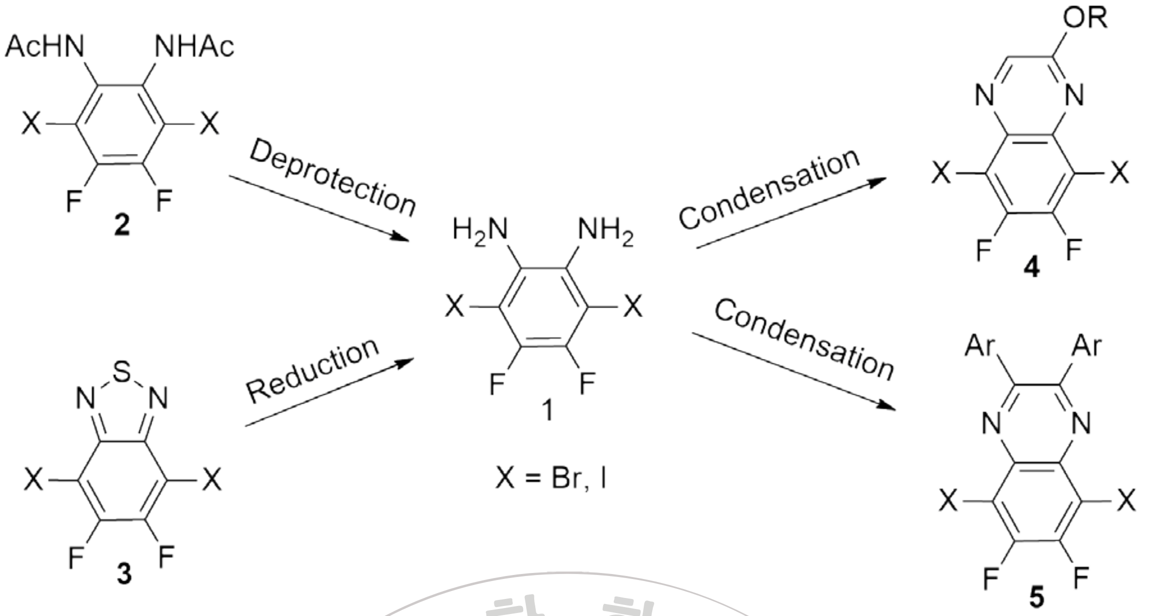
Poster Presentation : **ORGN.P-277**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Optical Properties of Multi-halogenated Quinoxaline Derivatives

Kyukwan Zong[*], **ShinYeong Kim**

Department of Chemistry Education, Jeonbuk National University, Korea

The D-A conjugated polymers containing quinoxaline unit have received a great attention in the field of organic photovoltaics because the devices formulated from them usually revealed high power conversion efficiencies.1 The donor polymers made from quinoxaline moiety are very attractive due to low cost and high performance for polymer donor materials for polymer solar cells. Most of quinoxaline monomers are synthesized through the reduction of 3 and followed by condensation with various diones.2 The starting material 3 is commercially expensive to purchase and thus synthesis starting from 3 suffers from high cost. In this presentation, we present a new route for synthesis of quinoxaline derivatives (4 and 5) from cheap starting material (2). Spectroscopic and optical properties of the compounds will be discussed. References1.Sun, C.; Zhu, C.; Meng, L.; Li, Y. Adv. Mater. 2021, 2104161.2.Zhu, C.; Meng, L.; Zhang, J.; Qin, S.; Lai, W.; Qiu, B.; Yuan, J.; Wan, Y.; Huang, W.; Li, Y. Adv. Mater. 2021, 2100474.


AcHN
NHAc
X
X
F
F
2
Deprotection
N
S
N
X
X
F
F
3
Reduction
H2N
NH2
X
X
F
F
1
X = Br, I
Condensation
OR
N
N
X
X
F
F
4
Condensation
Ar
Ar
N
N
X
X
F
F
5

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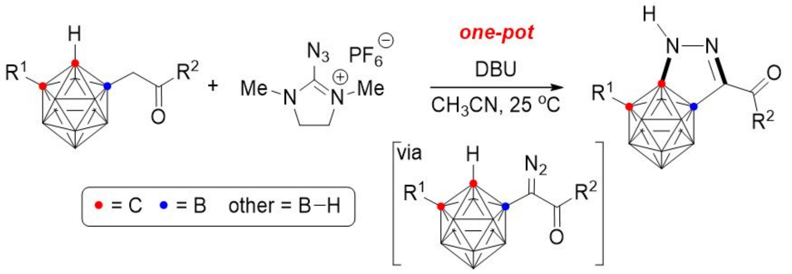
Poster Presentation : **ORGN.P-278**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthetic Methods of *o*-Carborane-Fused Pyrazoles via Sequential C-N Bond Formation

Gi Hoon Ko, Daesu Park, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

The characteristics of boron cluster, including aromaticity, unusual thermal and chemical stability, and synthetic robustness, make the carborane derivatives be a class of significant building blocks in pivotal frameworks in pharmaceuticals and BNCT, ligands in organometallic chemistry, and functional materials. To this end, the development of efficient methodologies for the facile synthesis of *o*-carborane-fused heterocycles is highly required. We have demonstrated an efficient synthetic method for *o*-carborane-fused pyrazoles as a new scaffold under transition-metal free conditions from the reaction of B(4)-acylmethyl and B(3,5)-diacylmethyl *o*-carborane with ADMP in the presence of DBU in acetonitrile through sequential diazotization and cyclization in one-pot. This method proceeded through two- or three-fold C−N bond formation under extremely mild conditions with high functional group tolerance.



☑ *o-carborane-fused pyrazoles*
☑ *sequential reaction in one-pot*
☑ *mild conditions*
☑ *metal-free*
☑ *good functioal group tolerance*
☑ *two-fold C−N bond formation*

Poster Presentation : **ORGN.P-279**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Practical Direct Synthesis of Anhydrides from Aldehydes using Dibromoisocyanuric Acid

Truong Giang Luu, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Carboxylic anhydrides are one of useful structures in organic compounds because of their wide utilization in chemistry including pharmaceutical industry. Therefore, development of efficient synthetic methods for carboxylic anhydrides is highly valuable. One of traditional methods to give carboxylic anhydrides is reaction of carboxylic acids with dehydrating coupling agents, which have several disadvantages including employment of unstable or challenging-to-handle reagents, complicated workup procedures, and limited scope. To overcome these limitations, many novel strategies were explored. One promising approach is utilization of alternative starting materials such as aldehydes. Herein, a novel one-pot synthesis of carboxylic anhydrides in mild conditions was reported. In the synthesis, dibromoisocyanuric acid was served as the source of bromine to produce in situ acyl bromides, that were further used to yield desired carboxylic anhydrides. Using this transformation, various carboxylic anhydrides were synthesized successfully in high yields at room temperature. The result indicated that this strategy is a promising method for the synthesis of carboxylic anhydrides.

Poster Presentation : **ORGN.P-280**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

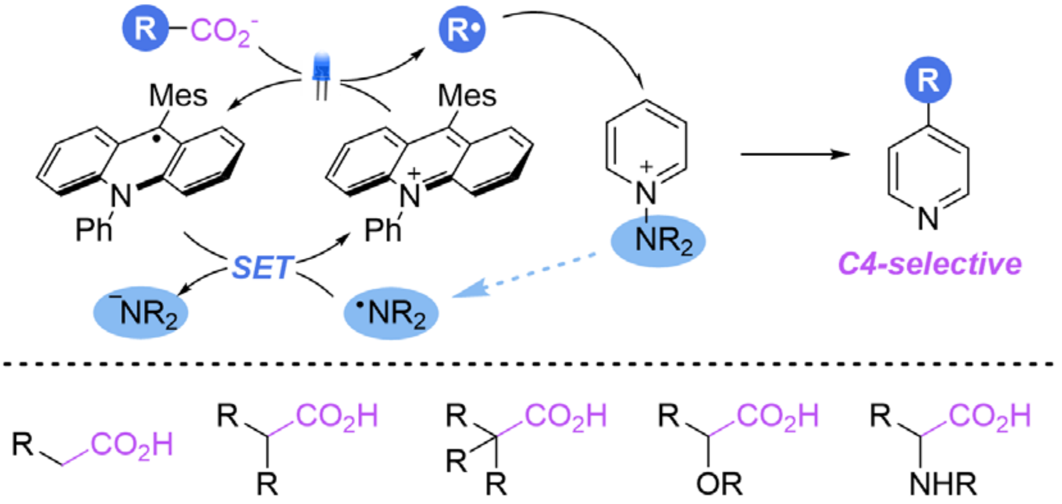
Photocatalytic Site selective Decarboxylative pyridylation of Alkyl Carboxylic acids

Jinwook Jeong, Sungwoo Hong[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Site-selective C−H functionalization of heteroarenes is essential for efficiently modifying bioactive molecules. In this work, we report an efficient photocatalytic strategy of the photo-induced C−H alkylation at the C4 position of pyridines using alkyl carboxylic acids as alkylating agents. Notably, the in situ-generated N-centered radical can act as an oxidizing agent to regenerate the photocatalyst via single-electron transfer (SET) oxidation. This photocatalytic system does not require an external oxidant for the reactions, and this successfully enables a broad substrate scope for pyridines and carboxylic acids containing oxidant-sensitive functionalities that are unsuitable for other procedures. The strategy provides an efficient platform for the C4-selective pyridylation with a diverse range of carboxylic acids and amino acids with various functional groups under mild conditions.



Poster Presentation : **ORGN.P-281**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Site-Selective Pyridine C–H Alkylation with Alcohols and Thiols via Single-Electron Transfer of Frustrated Lewis Pairs

Chang-Yin Tan

Korea Advanced Institute of Science and Technology, China

A new strategy for the selective pyridylation of alcohols and thiols, which involves the use of frustrated Lewis pairs (FLPs) derived from pyridinium salts and PtBu3. The FLPs are generated through a single-electron transfer (SET) process, and the alkyl radical is formed through the β-scission of the in situ generated xanthate. The efficiency of the reaction is further enhanced by visible-light irradiation.

Poster Presentation : **ORGN.P-282**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Visible-light-mediated synthesis of sulfonic esters via three component reaction using copper catalyst

Truong Giang Luu, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Sulfonyl ester is an important motif occurring in structure of many natural compounds as well as in pharmaceuticals. Therefore, the search for simple, efficient, and economic methods of synthesizing sulfonyl esters is receiving much attention from scientists. Recently, photochemical reaction has become an attractive research topic because of its advantages such as environmental friendliness, mild reaction conditions, and easy control. Besides, arylazo sulfones have also been shown to be an effective source in reactions involving free radical mechanisms. Herein, a visible-light-induced synthetic method to prepare aryl sulfonic ester from arylazo sulfones was presented. In the present study, a one-pot reaction using CuI and HCl to produce sulfonic esters was performed via three component reaction of arylazo sulfones, DABSO, and alcohols. This protocol provided novel synthetic approach to give sulfonic esters with high yields.

Poster Presentation : **ORGN.P-283**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

AFCPC-Composed Foldamers with New Characteristics: Synthesis and Characterization

Yisak Park, Jungwoo Hong, Hee-Seung Lee*

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

Proteins' structure and function are determined by amino acid sequence and secondary structure. To mimic protein function, β-peptide foldamers composed of trans-ACPC(2-aminocyclo-pentanecarboxylic acid) have been developed. In this study, we synthesized AOCPC(2-amino-4-oxocyclopentanecarboxylic acid) and AFCPC(2-amino-4,4-difluorocyclopentanecarboxylic acid) to introduce new chemical and structural characteristics to the foldamers. AFCPC, containing a difluoromethylene group, was used to investigate its effect on foldecture self-assembly. Scanning electron microscope analysis showed that the foldecture of the AFCPC-composed foldamer has the same C4v-symmetry as existing foldamers made of ACPC but appeared to have a different shape. We envision that the AFCPC-introduced foldamers will exhibit different characteristics in liquid systems than those made of ACPC due to the introduction of the difluoromethylene groups. This research may have important implications for developing new materials with specific functional properties.

Poster Presentation : **ORGN.P-284**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhancing the Functionality of Helical Peptidic Foldamers via a Biomimetic Approach

Minsang Kang, Hee-Seung Lee[*]

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

Foldecture, a 3D microstructure made up of peptidic helical foldamers, has been researched as a way to create structures with unique shapes and sizes. However, it has yet to reach the level of functional architecture seen in enzymes. To increase its functionality and versatility, adding functional groups to the amino acids was explored but only resulted in limited success in terms of surface modification for hierarchical assembly. In order to attain the catalytic functionality of Foldecture, it is crucial to design a precise introduction of functional groups into the peptidic foldamers, the building blocks of Foldecture. This study was informed by the active site of natural hydrolases, known as the catalytic triad, in creating a catalytic center for the peptidic foldamer. This center was simplified to a 'catalytic dyad' composed of hydroxyl group and pyridine on a peptidic foldamer scaffold for transesterification. However, it was determined after verification that only the pyridine ring served as the catalytic center. Further research will focus on designing a more precise catalytic dyad made up of hydroxyl and base to achieve a biomimetic catalytic foldamer and Foldecture.

Poster Presentation : **ORGN.P-285**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Fluorenones via intramolecular Friedel-Crafts Acylation

Yeji Shin, Hee Nam Lim*

Department of Chemistry and Biochemistry, Yeungnam University, Korea

Fluorenones, important chemical motifs in organic electronic materials and pharmaceuticals, were constructed by intramolecular Friedel-Crafts acylation using acyl fluorides as substrates. The transformation was successfully achieved by TMSOTf-mediated cyclization. The reaction was fast, chemoselective, and mild.

Poster Presentation : **ORGN.P-286**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Colorimetric Sensors of Various Biohazardous Metal ions Based on Polydiacetylenes

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Conjugated polymers known as polydiacetylenes (PDAs) have been studied as stimuli-responsive colorimetric and fluorometric chemosensors. Closely packed and ordered diacetylene monomers form alternating ene-yne polymer chains upon irradiation with 254 nm of UV light or with γ-irradiation. Disruption of the preferred ene–yne conjugated backbone promotes a blue-to-red color transition. Additionally, blue-phase PDAs with no-fluorescence can shift to become fluorescent in response to a stimuli, which facilitate the development of various chemosensors using the polymers. PDAs can selectively detect metals through metal binding and ionic interactions.We synthesized PCDA-HP and PCDA-IBA with the following strategy. PCDA-HP was synthesized with an HP-receptor composed of 5-hydroxy-N1,N3-bis(pyridin-2-ylmethyl)isophthalamide capable of detecting cadmium ions (Cd^{2+}). Addition of cadmium ions at both pH 7.4 and 6.8 results in selective and sensitive colorimetric and fluorometric changes. The PDA-HP was highly selective for cadmium ions over other metal ions with colorimetric changes. PCDA-IBA was synthesized by reacting N-(3-(1H-imidazol-1-yl)propyl)-4-hydroxybenzamide (IBA) as a chelating moiety. The PDA-IBA sensor exhibited selective colorimetric and zeta potential changes in the presence of silver ions (Ag^{+}). The most significant chromatic change was found for silver ions, since the absorption at 642 nm decreased and a new absorption band appeared at 520 nm, which could be attributed to the red-form of PDA. The change in PDA surface potential due to ion interaction was confirmed as zeta potential. As the equivalent weight of silver ions increases, oxidation of the surface of PDA occurs due to the reduction of silver ions, and Z-potential value increases.

Poster Presentation : **ORGN.P-287**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of disulfonylated m-terphenyl structure using copper-based catalytic system

Ji Hye Kim, Hee Nam Lim[*]

Department of Chemistry and Biochemistry, Yeungnam University, Korea

Aryl sulfide is a structure commonly found in drugs, polymers, and functional materials. Therefore, C-S bond forming reactions have received great attention in area of organic synthesis. In this study, efforts and results for synthesis of arylsulfones using 4,4''-dibromo-m-terphenyl and arylsulfinates under copper-based catalytic system are delineated.

Poster Presentation : **ORGN.P-288**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Manganese(I)-Catalyzed C-H Dienylation of Indoles and Cascade Cycloadditions

Jinhwan Park, Jongwoo Son[1,*]

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

1,3-Butadienes are widely utilized as building blocks for the construction of complex natural products and biologically active compounds containing cyclohexene scaffold via Diels-Alder cycloaddition. Conventionally, preparation of 1,3-butadienes is challenging due to their multiple reaction steps resulting in poor atom efficiency and cost-ineffectiveness. Moreover, a straightforward installation of 1,3-butadiene motif has rarely been reported. In this poster presentation, we describe manganese(I)-catalyzed C-H dienylation of indoles using allenyl esters as well as their cascade [4+2] cycloaddition to a variety of dienophiles. This protocol introduces excellent regioselectivity and functional group tolerance in a sustainable manner.

Poster Presentation : **ORGN.P-289**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Formal Synthesis of [18F]Rucaparib

Ju-Ahn Seo, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Rucaparib is PARP inhibitor used as an anti-cancer agent. It was approved by the Food and Drug Administration (FDA) in 2016 and 2020, respectively. To study the metabolic pathway of rucaparib, isotopologues capable of obtaining bio-images was developed. In particular, the [18F]-isotopologue of rucaparib, which can use available PET for certain metabolic tracings, could be formed from boronic ester precursor. However, since this compound follows the existing process chemistry route, they have limitations, such as lengthy synthetic steps and low yields.Recently, our group developed a highly efficient synthetic route for rucaparib from 2-aminocinnamic acid derivative and aldehyde using the cyanide-catalyzed imino-Stetter reaction as the key step to construct tetra-substituted indole intermediate. Based on these synthetic methods, a formal synthesis of [18F]rucaparib was developed. 2-Aminocinnamnitrile can be prepared by Heck coupling of a methyl 3-amino-2-iodobenzoate derivative with acrylonitrile. Imino-Stetter reaction of the resulting 2-aminocinnamnitrile derivative with an aldehyde provided the required tri-substituted indole-3-acetonitrile. Subsequent azepinone ring formation followed by installation of pinacol boronate completed the formal synthesis of [18F]rucaparib. In this poster presentation, the development of the formal synthesis of [18F]rucaparib will be discussed.

Poster Presentation : **ORGN.P-290**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of 2-(2-Nitrophenyl)indoline-3-acetic Acid Derivatives via Base-catalyzed Cyclization of N-Benzyl-2-aminocinnamic Acid Derivatives

Jong Mu Kim, Cheol-Hong Cheon[1,*]

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

Indoline, which is a partially reduced structure in the indole, has been identified as an important structural subunit for numerous natural products and bioactive compounds. As previous studies have confirmed that partial saturation of the core structure has various effects on biochemical activity, comparing the properties of indole indoline is a great interest of both synthetic and pharmacological communities. However, synthetic protocols to access indoline scaffold have remained far less unexplored, and this became an obstacle to research. In this poster presentation, we will introduce a three-step protocol to access 2-(2-nitrophenyl)indoline-3-acitic acid derivatives from N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives via base-catalyzed cyclization, and utility of indoline.

Poster Presentation : **ORGN.P-291**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Syntheses of All Regioisomers of Azaindole-3-acetic acid Derivatives Bearing C2-Aryl Group

Taewook Kim, Cheol-Hong Cheon[1,*]

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

Since azaindoles, compounds bearing a nitrogen atom in place of a carbon atom in the indole subunit, are common scaffolds found in many natural products, and display intriguing biological activities compared to the parent indole derivatives, the development of a novel protocol to access these azaindole has been considered the research of importance. However, methods to synthesize azaindole scaffold have been far less explored compared to the indole counterparts.Our group developed a highly efficient protocol for the synthesis of 2-aryl substituted indole-3-acetic acid derivatives via the cyanide-catalyzed imino-Stetter reaction of aldimines derived from 2-aminocinnamic acid derivatives and aromatic aldehydes. Since the imino-Stetter reaction applies a very broad substrate scope, we attempted to extend this protocol to the synthesis of 2-aryl azaindole-3-acetic acid derivatives from 2-amino-azacinnamic acid derivatives. In this poster presentation, we will disclose the development of a novel protocol for the synthesis of all regioisomers of 2-aryl azaindole-3-acitic acid derivatives via imino-Stetter reaction. The challenges and generality of this protocol will be discussed in this poster presentation.

Poster Presentation : **ORGN.P-292**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and analysis of oxadiazole energetic compounds

SeungHee Kim[*], Kuktae Kwon, So Jung Lee

Agency for Defense Development, Korea

Energetic compouds means that compounds release energy very fast when they decompose. Most well known ernergetic materials are explosives such as TNT(2,4,6-Trinitrotoluene) and RDX(Hexogen). TNT and RDX are using more than 100 years, so there were many tries to replace these old compounds. Recently, azole compounds are regarded as good candidates for next generation molecular explosives. It is because of their high heat of formation and low sensitivity. Oxadiazole compounds are branches of azole compounds and some of them showed superior energetic properties than common azole compounds. But synthetic pathways are complicated than traditional azole compounds. Here in, we describe synthesis and analysis of energetic oxadiazole compounds.

Poster Presentation : **ORGN.P-293**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

The combination of activatable sonosensitizer and immune stimulant imiquimod for immuno-sonodynamic therapy

Changyu Yoon, Jusung An, Ji Hyeon Kim, Jaewon Kim, Injun Lee, Jieun Lee, Yujin Kim, Huiyeon Moon, Jiyoung Yoo, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Sonodynamic therapy (SDT) has received a lot of interest as a noninvasive treatment for deep tumors. Compared to Photodynamic therapy (PDT), SDT achieves a higher tissue penetration by substituting ultrasonic for light. Additionally, the FDA-approved toll-like receptor 7 agonist imiquimod (R837) is frequently utilized in clinical settings as an immunological adjuvant. We developed an activatable sonodynamic sensitizer platform based on glutathione-sensitive disulfide bonds connecting Leu-MB, the reduced form of methylene blue (MB), and R837 to enable effective combinatory SDT and immunotherapy for cancers without hurting healthy tissues. Furthermore, we produced self-assembled MB-R837-PEG (MRP) nanoparticles for immunosonodynamic therapy (iSDT) using the amphiphilic polymer 18PMH-PEG. Our MRP showed a great sonodynamic effect selectively between the tumor cell and normal cell compared to SDT reported in the literature. The immune response was induced by the iSDT, which is performed through immune adjuvants released at the tumor site, and this enhances the treatment's ability to kill tumors. MRP was selectively activated by glutathione in the tumor microenvironment to release MB and R837, exhibiting excellent antitumor sonodynamic and immune responses. In addition, this treatment successfully prevented tumor metastasis when combined with an α-PD-L1 antibody for immune checkpoint blockage. Additionally, mice treated with MRP and α-PD-L1 antibody did not grow tumors even after a tumor reinoculation, showing that long-term immune memory had been acquired. This work presents the idea of sonodynamic sensitizer production as a next-generation iSDT based on a noninvasive synergistic therapeutic strategy that will be used in the near future.

Poster Presentation : **ORGN.P-294**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Self-assembled photoswitch in tandem with morphological modulation

Eunji Kim, Ji Hyeon Kim, Jusung An, Jungryun Kim, Jaewon Kim, Hyeonji Rha, Jieun Lee, Soyu Zi, Injun Lee, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Since the light-responsive switches have inspired their potential in various fields to utilize the binary properties in application, hydrazone is one of the candidates for performance. However, current systems carry limitations such as bistability, solubility in aqueous media and applicable absorbance wavelength of light source. Herein, we report morphological variations of a self-assembled photoswtich based on hydrazone derivatives. The reversibility supports nano-scale formal modulation and suggests accessible structure in response to visible light exhibiting On/Off fluorescence.

Poster Presentation : **ORGN.P-295**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

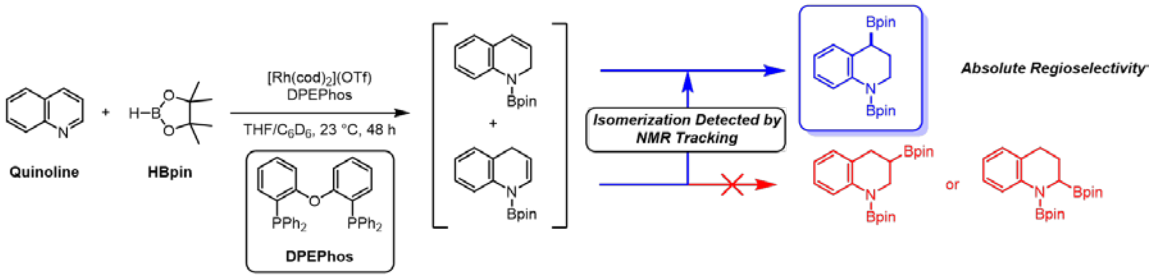
Mechanistic Understanding of Rhodium-catalyzed Selective Double Hydroboration of Quinoline

<u>Seung Hyun Lee</u>, Sehoon Park[1,*], Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Chemistry, Guangdong Technion Israel Institute of Technology, China*

Tetrahydroquinoline (THQ) is a common structural motif found in natural products and widely used in medicinal chemistry. To tailor its properties for specific applications, chemists have developed several approaches to synthesize functionalized THQ. The hydroboration of THQ is considered one of the most efficient methods, as it provides a synthon that can be readily functionalized with a high degree of tolerance. The Park group has recently developed Rh-catalyzed hydroboration of N-heteroarenes, including the first report on the double hydroboration of pyridine.[1] Despite their success in asymmetric and site-selective double hydroboration of pyridine with extensive experimental investigations, the absolute regioselectivity for the THQ still remained unclear. In this study, we performed density functional theory calculations to gain a deeper understanding of the reaction mechanism and provide a detailed analysis on the absolute regioselectivity of double hydroboration on the quinoline. Our results show that the unprecedented chelate isomerization plays a key role in determining the regioselectivity. This study not only enhances our understanding of the reaction mechanism but also provides an efficient platform for the atom-economic synthesis of THQ derivatives that could greatly benefit the pharmaceutical and synthetic chemical fields.



Poster Presentation : **ORGN.P-296**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Application and Characterization of Polydopamine (PDA) Film Inspired by Mussels

Joowon Choi, Kyungtae Kang[*]

Department of Applied Chemistry, Kyung Hee University, Korea

The polydopamine (PDA) film inspired by mussels has shown tremendous potential as a material, thanks to its easy synthetic process and reliable substrate-independent surface deposition. Melanin is produced through a series of chemical reactions that start with the hydroxylation of tyrosine using 3,4-dihydroxyphenylalanine (DOPA), followed by dopaquinone and dopachrome. Dopachrome is then converted into indole-5,6-quinone after being decarboxylated to 5,6-dihydroxyindole and rapidly oxidized. The decarboxylation process may be affected by the presence of certain metal ions or enzymes, leading to the formation of eumelanin. When dopaquinone is mixed with cysteine, it forms reddish-yellow pheomelanin showing many interesting materials properties distinct from eumelanin. Inspired by pheomelanin, we tried to design thin films made of dopamine and L-cysteine esters. The film was exceptionally thin (< 10 nm), as opposed to conventioanl eumelanin-like films (which are typically thicker than 50 nm), and surprisingly, was able to catalyze the oxygen evolution reaction (OER) highly effectively. We used various analytic methods to investigate the newly found film and its deposition process.

Poster Presentation : **ORGN.P-297**

Organic Chemistry

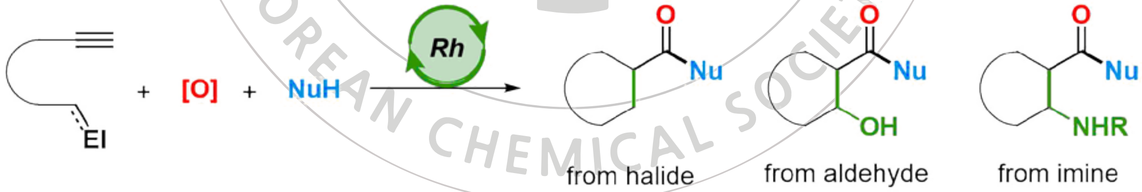
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Carbofunctionalization of Terminal Alkynes via Combined Rhodium Catalysis Enabling Formations of Four Different Bonds

Dae-Kwon Kim, 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-298**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Molecular Design Strategy for Realizing Vectorial Electron Transfer in Photoelectrodes

Deok-Ho Roh, Tae-Hyuk Kwon*

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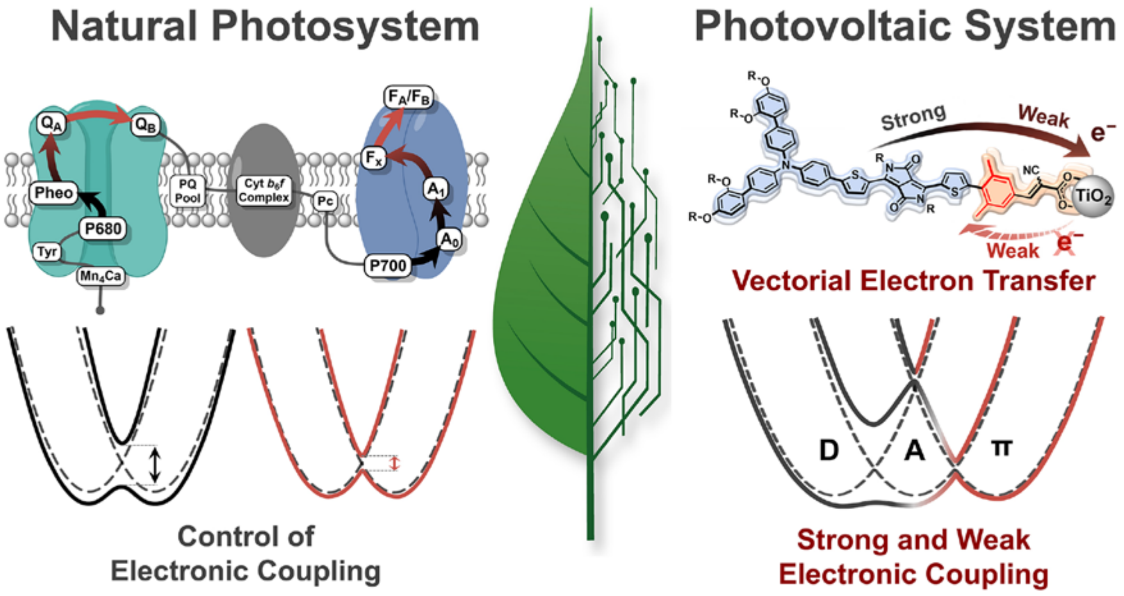
Vectorial electron transfer is essential for developing ideal artificial photosystems. Conventional photosensitizers with only strong electronic coupling, as used in photovoltaics, cannot achieve vectorial electron transfer because of their rapid charge recombination. Herein, we present a design strategy for integrating strong (~600 cm−1) and relatively weak (310 cm−1) electronic coupling in a single molecule to realize vectorial electron transfer in dye-sensitized solar cells. Four sensitizers with donor–acceptor–π-spacer and anchoring group configurations are developed, and the electronic coupling in these sensitizers is controlled by the π-spacers of varying steric hindrances. Transient-absorption spectroscopies reveal the occurrence of vectorial electron transfer in the designed sensitizer by suppressing charge recombination via weakened electronic coupling between the acceptor and π-spacer and efficient charge injection via strong electronic coupling between the donor and acceptor. The optimization of electronic coupling in the sensitizers improves the photovoltaic performances, achieving a power-conversion efficiency of 10.8%.


Natural Photosystem
Photovoltaic System
Q_A
Q_B
Pheo
P680
Tyr
Mn_4Ca
PQ Pool
Cyt b_6f Complex
Pc
F_A/F_B
F_X
A_1
A_0
P700
Strong
Weak
e^-
Weak
e^-
NC
TiO_2
Vectorial Electron Transfer
D
A
π
Control of Electronic Coupling
Strong and Weak Electronic Coupling

Poster Presentation : **ORGN.P-299**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Strategy for Reducing Non-radiative Recombination in Dye-sensitized Solar Cell

Seungrok Kim, Tae-Hyuk Kwon[1,*]

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[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 have focused on reducing the radiative recombination, and research to reduce the non-radiative recombination are less investigated. Herein, this research propose 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. 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. We expect this work contribute to molecular strategy understanding isotope effect on recombination process.

Poster Presentation : **ORGN.P-300**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Non-canonical pyroptosis triggered by photocatalytic oxidation of intracellular membranes

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

Gasdermin-driven pyroptosis, a lytic programmed cell death, is a signal inducing substantial inflammatory and immune responses. However, pyroptosis-inducing chemical factors remain fully unexplored. Herein, we demonstrate that photocatalytic membrane oxidation triggers pyroptosis. An amphiphilic photocatalyst oxidatively damaged membranes by generating hydroxyl radicals and hydrogen peroxides via water oxidation, which was accelerated under hypoxia. Experimental results using single-molecule magnetic tweezers revealed that photocatalysis-induced oxidation markedly destabilised membrane protein folding. Label-free quantification revealed that oxidative damage occurred primarily in membrane proteins related to protein quality control, thereby aggravating mitochondrial and endoplasmic reticulum stress and inducing lytic cell death. Notably, photocatalysis activated non-canonical inflammasome caspases, resulting in gasdermin D cleavage to its pore-forming fragment and subsequent pyroptosis. These findings propose a photochemical approach to spatiotemporally manipulate non-canonical pyroptosis.

Poster Presentation : **ORGN.P-301**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

New detergents for nanodisc formation with membrane proteins

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Department of Bionano Engineering, Hanyang University, Korea

Membrane proteins are implicated in various diseases and are thus main targets for many pharmaceutics. Information on membrane protein structures are important in drug discovery, but structure determination of membrane proteins is highly challenging due to the instability of these bio-macromolecules in an aqueous environment. Detergent micelles are most widely used as a membrane-mimetic system for in vitro study of membrane proteins. However, membrane proteins encapsulated in detergent micelles are often unstable, making them unsuitable for downstream characterization. Recently, an alternative membrane-mimetic system, called nanodiscs (NDs), has received tremendous attention due to its enhanced mimicry of native membranes. Current technology requires large proteins or polymers to construct NDs with membrane proteins, which limits utility of this membrane mimetic system. In the current study, we introduce a couple of detergents with the ability to form NDs with liposome and cell membranes. These detergents, derived from previously developed glucose neopentyl glycols (GNGs), contain a fluorinated chain in the lipophilic region. Preliminary result showed that the incubation of these detergents with DMPC vesicles and cell membranes resulted in the formation discoidal self-assemblies, as evidenced by TEM image. As the new detergents have the ability to extract membrane proteins from the membranes in a nanodisc form and their properties can be further optimized via structural modification, these detergents hold significant potential for membrane protein structural study

Poster Presentation : **ORGN.P-302**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Hydrophobicity tailoring of small molecule probes for subnanomolar-sensitive detection of Aβ in Alzheimer's disease mouse brain

Soyu Zi, Ji Hyeon Kim, Jusung An, Jungryun Kim, Hyeonji Rha, Eunji Kim, Injun Lee, Yujin Kim, Changyu Yoon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

The pathological origin of Alzheimer's disease (AD) is still shrouded in mystery. The selective visualization of β-amyloid (Aβ), the most abundant proteinaceous deposit, is pivotal to revealing AD pathology. Unlike enzymes or receptors with specific binding sites, Aβ is an atypical protein exhibiting less predictable binding modes with small-molecular ligands. The Aβ has the structural characteristic “cross-β-sheet” scaffold, in which adjacent chain segments are tightly folded in an anti-parallel way within the fiber lattice. Based on the intrinsic hydrophobicity of Aβ, small molecule dyes have been postulated to bind *via* hydrophobic π-π stacking interactions to these β-sheets surfaces or intercalate into hydrophobic grooves and channels.To date, several small-molecule fluorophores for Aβ have been developed with increasing binding affinities through enhancing hydrophobicity. However, the increased hydrophobicity associated with an extended π-conjugation inevitably leads to poor aqueous solubility and induces the ligands’ promiscuity regarding other hydrophobic proteins and cellular components. Thus, the major challenge in designing new red-emissive dyes with a stronger affinity for Aβ fibrils is maintaining adequate aqueous solubility specificity, and sensitivity.In this work, small-molecular dioxaborine-derived dyes were rationally designed by tailoring the hydrophobicity to enhance the binding affinity for Aβ$_{1\text{-}42}$ fibrils —while concurrently preventing poor aqueous solubility—*via* biannulate donor motifs in D-π-A dyes. An unprecedented sub-nanomolar affinity was found ($K_d = 0.62 \pm 0.33$ nM) and applied to super-sensitive and red-emissive fluorescent staining of amyloid plaques in cortical brain tissue ex vivo.

Poster Presentation : **ORGN.P-303**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Acid-Responsive Nanoporphyrin Evolution for Near-Infrared Fluorescence-Guided Photo-Ablation of Biofilm

HyunSun Jeong, Hee Jeong Kim, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Pathogenic bacteria infection induced a lot of progress in antibiotics. However, controlling biofilm infections still remains a challenge due to its special structural protection and acidic conditions. Herein, we constructed an acid-responsive nanoporphyrin (PN3-NP) based on the self-assembly of a water-soluble porphyrin derivative (PN3). The introduction of amino groups by conjugation of spermine units to porphyrin macrocycle provided additional kinetic control sites, which made PN3 self-assemble into stable nanoparticles (PN3-NP) under physiological environment. Notably, the transformation of the nanoparticles into dot-like nanospheres triggered by the acidity in biofilm, turned on near-infrared (NIR) fluorescence monitoring and synergistic phototherapeutic effects of PN3-NP. Thus, we could effectively minimize the normal tissue damage and successfully achieve precise diagnosis and treatment of biofilms. The results of fluorescence imaging guided photo-ablation of anti-biotic resistant strains methicillin-resistant Staphylococcus aureus (MRSA) biofilms demonstrated that PN3-NP could be a ideal alternative to antibiotics, as a photosensitizer. Meanwhile, this strategy also provides facile approach and new horizons to design smart nano-photosensitizer for accurate diagnosis and treatment of biofilms.

Poster Presentation : **ORGN.P-304**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Hexa-BODIPY-cyclotriphosphazene based nanoparticle for NIR fluorescence/photoacoustic dual-modal imaging and photothermal cancer therapy

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Ewha Womans University, Korea

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

Theranostic is drawing attention as a cancer treatment strategy that enables simultaneous diagnosis and tumor treatment. Here, we have devised a new teranostic nanoparticle based on hexa-body pycrophosphazene. Because HBCP has a large molecular structure, HBCP NPs can simultaneously perform near-infrared fluorescence imaging and photoacoustic imaging. In addition, the generation of reactive oxygen species is completely inhibited even under laser irradiation, which has the advantage of being able to perform safe fluorescence imaging without the risk of cell damage. A study performed in 4T1 tumor-bearing mice shown that in vivo NIR fluorescence imaging and PAI are possible in tandem, also it showed selective accumulation at tumor area. Finally, irradiation of high-power laser effectively distrupt tumor growth in mice, suggesting that HBCP NPs have a great potential as dual imaging- guided PTT nanoparticles.

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Poster Presentation : **ORGN.P-305**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

GLUT1-targeted pinpoint sonodynamic therapy for Rheumatoid Arthritis

Jaewon Kim, Ji Hyeon Kim, Le Yu, Jusung An, Jungryun Kim, Hyeonji Rha, Jieun Lee, Eunji Kim, Injun Lee, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Sonodynamic therapy (SDT) has garnered extensive attention as a noninvasive treatment for deep tumors. We envisioned that new design of an activatable sonosensitizer platform based on ascorbate as a GLUT1-targeting moiety (A-MB) and methotrexate (MTX) as an anti-rheumatoid arthritis drug conjugated Leu-MB (MTX-MB). First, we focused on the comparison anti-rheumatoid arthritis efficacy between A-MB and MTX-MB after hydrolyzing to methylene blue (MB) on-site and releasing MTX from MTX-MB to achieve efficient combinatory SDT for tumors without harming normal tissues. To accomplish these strategies, we adopt the peroxynitrite ($ONOO^-$) and hypochlorite ($HOCl^-$) responsive group on our molecular design due to the double-targeting effect. The concept of sonosensitizer preparation as a next-generation SDT based on a noninvasive and pinpoint combinatorial therapeutic modality applicable in the near future is presented in this study.

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Poster Presentation : **ORGN.P-306**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Short peptide based Amyloid fibers that exhibit PLP-based covalent catalysis

Joonhyun Bae, Kyungtae Kang[1,*]

Department of applied chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Pyridoxal-5-phosphate (PLP) governs a wide variety of chemically demanding reactions, such as decarboxylation, racemization, and transamination. When coupled with an amine, PLP forms an imine intermediate, which has a shallow energy landscape that can undergo a group of reactions simultaneously. In a diluted solution, this makes PLP-catalyzed reactions extremely non-selective. Moreover, PLP-imine intermediates are prone to being hydrolyzed back to PLP. In this study, we investigated whether lysine-displaying amyloid fibers could capture PLP and use it as a cofactor for catalysis in a selective manner. The fibers were made of a set of sequence-variable short peptides, which allowed us to control the surface-exposed residues.

Poster Presentation : **ORGN.P-307**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Three-Component Coupling Reactions Involving Arynes, Phosphites, and Aldehydes toward 3-Mono-substituted Benzoxaphosphole 1-oxides

Hanbyeol Kim

Sogang University, Korea

A mild, efficient, and transition-metal-free three-component coupling reaction involving arynes, phosphites, and aldehydes was established to afford 3-mono-substituted benzoxaphosphole 1-oxides. A range of 3-mono-substituted benzoxaphosphole 1-oxides was obtained from both aryl- and aliphatic-substituted aldehydes in moderate to good yields. Moreover, the synthetic utility of the reaction was demonstrated by a gram-scale reaction and the transformation of the products into various P-containing bicycles.

Poster Presentation : **ORGN.P-308**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthetic Strategy for Aryl(alkynyl)phosphinates by a Three-Component Coupling Reaction Involving Arynes, Phosphites, and Alkynes

Suhyun Ji

Sogang University, Korea

An efficient and straightforward method for the synthesis of aryl(alkynyl)phosphinates was developed via a three-component coupling reaction involving arynes, phosphites, and alkynes. An array of aryl(alkynyl)phosphinates were produced from both aryl and aliphatic group-substituted acetylenes. This operationally simple reaction is tolerant to many functional groups, affording various aryl(alkynyl)phosphinates in moderate to good yields. The synthetic utility of alkynyl phosphinates afforded by this method was demonstrated by the elaboration of the products into various phosphorus-containing compounds.

Poster Presentation : **ORGN.P-309**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Progress Toward the Total Synthesis of Aristolactams CII and DII

Jeong Min Bak, Inji Shin[1,*], Hee Nam Lim[*]

Department of Chemistry and Biochemistry, Yeungnam University, Korea
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Synthetic studies toward total syntheses of Aristolactams CII and DII, naturally occurring phenanthrene lactam alkaloids, are described in the presentation. While several total syntheses of aristolactam family were reported, the synthesis of target compounds with unique substitution patterns at C2, C3, and C4 position (CII C2, C4=OMe, C3=CH2OH, DII C2=OH, C3=CO2H, C4=OMe) has not been achieved. We present a new synthetic route using deconstruction-construction strategy to aristolactams CII and DII.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-310**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of unsymmetrical carbonyl compounds via isocyanate intermediates

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[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Although unsymmetrical carbonyl compounds can be accessed by activated CO equivalents such as phosgene, triphosgene, CDI, activated carbonates, etc., reliable and environmentally benign synthetic protocols for unsymmetrically substituted carbonyl compounds are still an area of great interest. We recognized α-oximinopyruvates as a useful and safe carbonyl source for the synthesis of unsymmetrical ureas, carbonates, thiocarbonatates, carbamates and thiocarbamates. One-pot reaction using α-oximinopyruvates was discovered and it enabled synthesis of various carbonyl compounds.

Poster Presentation : **ORGN.P-311**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of on/off fluorescent probe for tracking hNQO1 with high signal-to-noise ratio

Min Hee Lee*, Ja Young Son[1]

Department of Chemistry, Sookmyung Women's University, Korea

[1]*Department of Chemistry, Sookmyung Women′s University, Korea*

Human NAD(P)H: quinone oxidoreductase 1 (hNQO1) is an antioxidant enzyme. And it works as a two-electron reductase responsible for detoxifying quinones by utilizing NAD(P)H as a cofactor. The past decades have witnessed great interest in monitoring intracellular NQO1 activity by developing fluorescent probes, which harbor various fluorophores coupled with a trimethyl lock quinone (TLQ) moiety as the response site.And, some literatures have reported that the hNQO1 activity increases under hypoxic cancer.In our research, we aimed to develop the on/off fluorescent probe 1 for detecting hNQO1 with high signal-to-noise ratio. A series of probes containing the TLQ moiety was devised and synthesized. Briefly, our probe showed fluorescence emission at 540 nm in the presence of hNQO1 and NADH under physiological condition. We will demonstrate the detection ability of probes and their potential biological application. This work is ongoing, and we expect our probe can be applicable to hNQO1-associated disease model.

Poster Presentation : **ORGN.P-312**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of small molecule fluorescent probe to visualize H_2S and NTR in various 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-313**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Bimodal recognition ability of fluorescent probe enables precise detection

Songyi Yoo, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Cancer growth and proliferation usually accompanies hypoxia, which increases drug resistance and reduces the effectiveness of expensive anticancer drugs. Recently, to solve this problem, various prodrugs, which have no drug effect in normal cells but show drug efficacy when cancer is expressed, are being studied. In particular, nitroreductase (NTR) and Human NAD(P)H quinone oxidoreductase-1(hNQO1) enzyme are oxidoreductases that use NAD(P)H as a coenzyme and, they are overexpressed in cancer cells. Because of these features, NTR and hNQO1 based enzyme reactions are being used for prodrug activation. However, there is no assay method that simultaneously detects NTR and hNQO1. In this study, we devised a new fluorescent probe that can provide a fluorescence change in response to the coexistence of NTR and hNQO1 under physiological conditions. We worked on synthesis of the probe and investigation of its photophysical properties, and further validation of the detection capability in living systems will be performed.

Poster Presentation : **ORGN.P-314**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A dual-emissive fluorescent probe based on an ICT-FRET mechanism for H2S detection

Na yoon Kim, Min Hee Lee*

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 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 combination of intramolecular charge transfer (ICT) and fluorescence resonance energy transfer (FRET) mechanisms. This study is ongoing, and we expect this probe can be applicable to detect H2S in various analytical conditions.

Poster Presentation : **ORGN.P-315**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Dual-site fluorescent probe for the simultaneous detection of ATP and HOCl using two different excitation wavelengths in aqueous solution.

Fortibui Maxine mambo, Min Hee Lee[1,*]

Chemistry, Sookmyung Women's University, Korea
[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Dual sensing has emerged as a potential tool to investigate the interaction between biological species. Probe 1 was successfully designed as a dual fluorescence sensor to simultaneously detect the presence of ATP and HOCl using two different channel (λex = 520 nm, λex = 420 nm respectively) equipped with two different active sites. The spirolactam ring of the rhodamine moiety undergoes ring opening in the presence of ATP while the thiomorpholine moiety is oxide upon addition of HOCl. The probe displayed low detection limit for both ATP and HOCl (4.13μM and 0.10 μM) respectively which can be used to detect both biological species at low concentrations. The probe showed high water solubility which is very advantageous in cell imaging.

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Organic Chemistry

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Selective Eradication of Cancer Stem Cells via UCP2 Targeted H^+-Transport Modulation on the Inner Mitochondrial Membrane

Jiyoung Yoo, Ji Hyeon Kim, Jusung An, Jaewon Kim, Jungryun Kim, Eunji Kim, Changyu Yoon, Huiyeon Moon, Yujin Kim, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Cancer stem cells (CSCs) are closely correlated to invasion and metastatic recurrence of various cancers. However, current cancer therapies are confined only to targeting the bulk of primary tumor cells, struggling with selective CSCs eradication. Here, we report a new proton (H^+) modulation method to remove the CSCs selectively via blocking the H^+ leaks on the inner mitochondrial membrane (IMM). In this regard, a multimodal molecule channel blocker with high biocompatibility, namely, Bo-Mt-Ge, is developed. Significantly, in this contribution, we successfully demonstrate that mitochondrial uncoupling protein UCP2 is related to the stemness of CSCs, which may offer a new insight for selective CSC drug discovery. Mechanistic studies showcase that Bo-Mt-Ge can specifically downregulate the UCP2 activities, block the leaks of the mitochondrial H^+, destruct the mitochondria membrane potential, and deplete the endogenous GSH, which constitute a unique mode of action synergistically activating apoptotic CSC death. Interestingly, Bo-Mt-Ge also overcomes the cancer therapeutic resistance via a two-pronged tactic: downregulation of drug efflux pump, P-glycoprotein and inhibition of antiapoptotic factor (e.g., Bcl-2). With these advantages, Bo-Mt-Ge proved to be one of the safest and most efficacious anti-CSC agents, with ca. 100-fold more potent than genipin alone in vitro and in vivo. This study offers new perspectives and promising solutions for future CSC therapies in the clinic.

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Poster Presentation : **ORGN.P-317**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Electrochemical synthesis of 4-thionucleoside analogues

Eunsil Kim, Guldana Issabayeva[1], Hyemi Jo[2], Song Jiho[3], Jiyoung Hyun[4], Seongyun Choi[1], Hwan Jung Lim[5,*], Duck-Hyung Lee[*], Seong Jun Park[5,*]

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[1]*medicinal chemistry and pharmacology, University of Science & Technology, Korea*
[2]*Chemistry, Yonsei University, Korea*
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[4]*data convergence drug research center, Korea Research Institute of Chemical Technology, Korea*
[5]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Over the past few decades, various nucleoside analogs with antiviral and anticancer properties have been discovered and investigated. One of the important chemotypes in this field is 4'-Thionucleosides, which have the oxygen in the furanose ring replaced by sulfur. For instance, Brivydine (BVDU), an inhibitor of herpes simplex virus (HSV) type 1, is rapidly metabolized by phosphorylase. However, its sulfur analog, 4'-thio BVDU, was resistant to phosphorylase, and showed a higher chemotherapeutic index than BVDU. 4'-Thionucleosides are normally synthesized from sulfoxide and nucleobase by the Pummerer reaction. However, the Pummerer reaction requires harsh reaction conditions and the utility of highly toxic reagents that limit its substrate scope. Herein, we made an attempt to synthesize α-CH(sp^3) substituted sulfides via an environmentally friendly electrochemical protocol that provides regioselective control of the synthesis under mild reaction conditions.

Poster Presentation : **ORGN.P-318**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of fluorescent probe for dual sensing hNQO1 and NTR in hypoxic cancer cells

Sojin Hong, Min Hee Lee*

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-319**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhanced Nucleophilic Substitution Reaction in Non-polar media with Crown-Calix[4]arenes as a Phase-Transfer Catalyst.

Yong Kwon Kim, Taehyun Park, Siwoo Lee, Su Yun Lee[1], Dong Wook Kim[1,*]

Department of chemistry, Inha University, Korea

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

When using alkali metal salts (eg., KF, CsF) for SN2 reactions, polar aprotic solvent is more suitable than non-polar solvent as they selectively dissolve metal cations. Additionally, phase-transfer catalyst (PTC) plays a key role in the SN2 reaction since it transports polar reagents to organic phase.In our previous work, we reported modern phase transfer catalysts, bis-triethylene glycolic crown-5-calix[4]arene (BTC5A) and bis-triethylene glycolic crown-6-calix[4]arene (BTC6A). Such multifunctional catalysts include a crown-calix moiety and ethylene glycols having terminal OH groups. The crown-calix[4]arene unit captures metal ions, and the terminal OH groups of the glycols stabilize the transition state of the SN2 reaction through interaction with the ‘naked fluoride’. As mentioned earlier, non-polar solvents are known to be unsuitable for SN2 fluorination using alkali metal fluoride, but this study identified that they show better performance in SN2 reaction in the presence of calix[4]arenes PTC. Kinetic studies were performed on substrates with mesylate leaving group to investigate the effect of solvent, and reaction rate was compared according to the polarity of the solvent. Catalyst-promoted fluorination was also carried out on 12 types of substrates used as natural products or drugs. As a result, it was confirmed that the reaction rate was about three times faster than that of the polar solvent in low molecular weight non-polar solvents such as hexane, and the reaction was completed in 15 minutes in the fast case.

Poster Presentation : **ORGN.P-320**

Organic Chemistry

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Chirality selectivity of anion-caiton coacervate droplets by liquid-liquid phase separation

Seongyun Park, Kyungtae Kang[*]

Department of Applied Chemistry, Kyung Hee University, Korea

Liquid-liquid phase separation (LLPS) is associated with most cellular processes, including stress response, signal transduction, gene expression, and protein aggregation. Its molecular level-mechanism(s), however, remains incompletely understood. In this study, chiral polymers were used as one of the components that undergo liquid-liquid phase separation (LLPS) to examine the functions of the resulting liquid coacervates in terms of chiral catalysis. We identified specific conditions under which various chiral scaffolds can form coacervates and studied the properties of these coacervates, including their ability to enrich chiral guests, such as biomolecules and organic small molecules, and catalyze asymmetric reactions within the coacervate phase.

Poster Presentation : **ORGN.P-321**

Organic Chemistry

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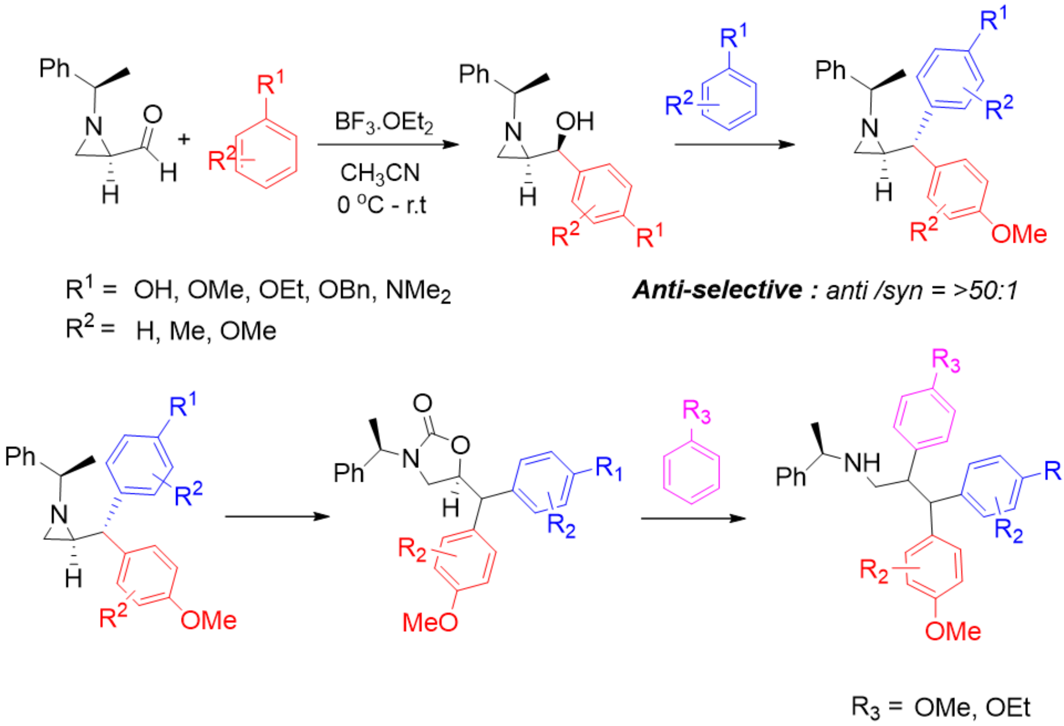
stereoselective bis-arylation and oxazolidinone-mediated stereoselective tris-arylation from aziridine-2-carboxylate.

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*

By demonstrated a Lewis acid-mediated stereoselective dehydroxylative cross coupling of aziridyl benzyl alcohols and electron-rich arenes, bisaryl aziridine with two different aryl group was composed. especially, when using electron-rich arene with a hydroxyl group at C3, a furan ring containing two different aryl group was composed simultaneously with aziridine ring opening. Next, oxazolidinone mediated streoselective synthesis of 2,3,3-tris-arylpropane-1-amine which has total three different aryl group was developed. this study proceed by one-pot synthesis of oxazolidinone and its ring opening in mild condition. this strategy offer unique and novel amine-containing molecules which can be important chiral center building block.


BF3.OEt2
CH3CN
0 °C - r.t
R1 = OH, OMe, OEt, OBn, NMe2
R2 = H, Me, OMe
Anti-selective : anti /syn = >50:1
R3 = OMe, OEt

Poster Presentation : **ORGN.P-322**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Pyridoquinolones: Bipolar Organic Molecules for Symmetric Redox Flow Batteries

Younghun Kim, Hyein Im, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Redox flow batteries (RFBs) represent an emerging technology for large-scale and rechargeable energy storage. One crucial drawback in implementing RFB is the crossover between the catholyte and anolyte, which compromises the cyclability of the cell. This problem can be addressed by symmetric RFBs employing bipolar molecules as both catholyte and anolyte. For this purpose, we have developed a new class of bipolar redox-active compounds featuring a polyheterocyclic core fused with pyridone and quinolone. The nitrogen atoms and carbonyl groups of these pyridoquinolones function as oxidation and reduction sites, respectively, the redox property of which can be modulated systematically by the substituents. With high modularity in synthetic design, various functional groups and solubilizing groups are readily installed onto the pyridoquinolone platform to prepare RFB electrolytes. This presentation will discuss the design principles, synthesis, and electrochemical properties of pyridoquinolone derivatives for potential applications in symmetric RFBs.

Poster Presentation : **ORGN.P-323**

Organic Chemistry

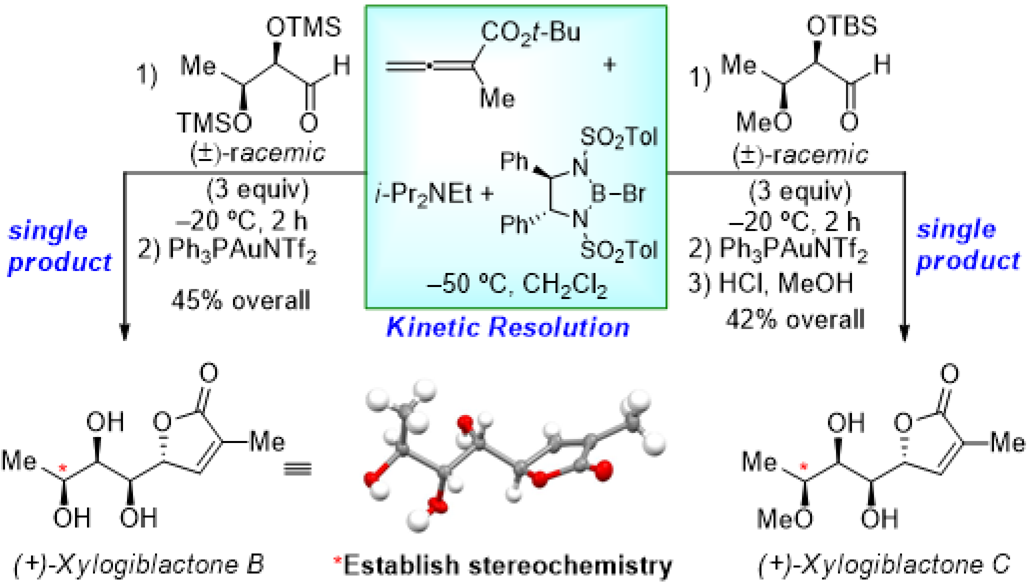
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Stereochemical Revision of (+)-Xylogiblactone B and C through a Kinetic Resolution of the Allenoate gamma-Addition

Jisu Kim, Suh Young Yu, Jihye Lee, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Regulating regio- and stereochemical pathway in organic reactions is one of the most important tasks in our laboratory. In this light, we recently disclosed a novel method for a kinetic resolution through the asymmetric gamma-addition of allenoates to racemic aldehydes. The method was proven to be effective resulting chiral 4-hydroxyallenoates bearing both axial and center chiralities as a single regio- and stereoisomer for all cases. We also demonstrated the method was applied not only in the syntheses of naturally occurring gamma-butenolides, (+)-xylogiblactone B and C but also in the correction of stereochemistry of the natural lactones. Herein, we will present key findings during the syntheses of (+)-xylogiblactone B and C.



Poster Presentation : **ORGN.P-324**

Organic Chemistry

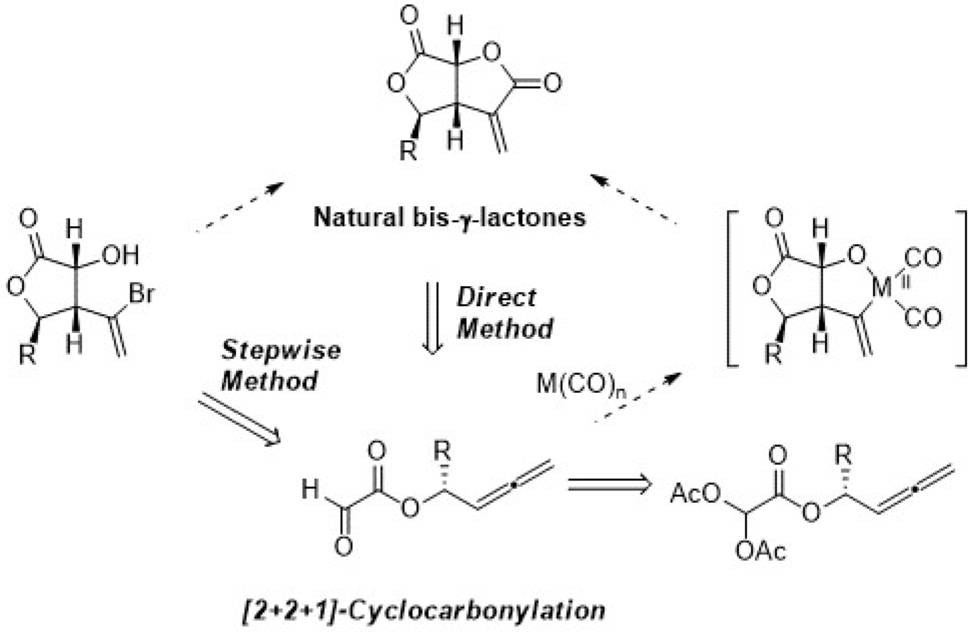
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Concise Syntheses of Bislactones from Allenyl Glyoxylates

Hyeonjoung Choi, Seyeon Jung, Zhang Aimin, Jimin Kim[*]

Department of Chemistry, Chonnam National University, Korea

Our efforts towards developing novel synthetic methodology continue to overcome challenges in the rapid construction of complex target molecules. The objective is to access complexity with a desired stereochemistry from rather simple starting materials. In this perspective, we have concentrated on a [2+2+1]-cyclocarbonylation using an allenyl component with two other pi-units to build a bislactone moiety. Herein, we will discuss the key findings in the cyclization event of allenyl glyoxylate and its utility for the synthesis of (-)-avenaciolide.



[2+2+1]-Cyclocarbonylation

Poster Presentation : **ORGN.P-325**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Size-dependent properties of melanin-like particles

Gaeun Kim, Kyungtae Kang[1,*]

Applied chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Melanin, a pigment that determinates a human skin color and its protective functions, is biosynthesized by enzymatically oxidizing tyrosine in a melanocyte. In melanin biosynthesis, the relative composition of the monomers, such as 5,6-dihydroxyindole, its carboxylic acid derivative, and others, largely determines the properties of melanin. Melanin-like particles (MLPs), also called polydopamine nanoparticle, can be prepared by adding a solution containing dopamine to a mixed solution of water-ethanol in the presence of ammonium hydroxide as a catalyst. In this process, the quantity of ammonium hydroxide is known to be used for controlling the size of MLPs. In this poster, we comparatively analyzed MLPs of different sizes focusing on their properties including UV-Vis absorbance, DPPH radical scavenging activity, atomic composition, and morphology. We expect that this will allow us to synthesize MLPs whose materials properties are fine-tuned for being applied as thin files, sensing platform, and theranostic devices.

Poster Presentation : **ORGN.P-326**

Organic Chemistry

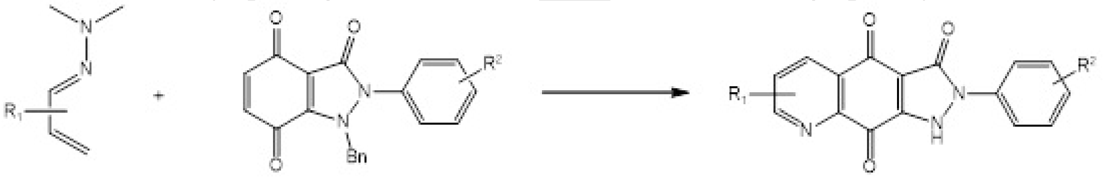
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Pyrazolone-fused azanaphthoquinone derivatives via Diels-Alder Reactions

Eunseon Yang, **Jeong Ho Kim**[1], **Hakwon Kim**[1,*]

department of applied chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Naphthoquinone (NQ) and pyrazole or pyrazol-3-one, respectively, have been known to have various physiological activities. In our previous study, N-substituted indazol-3,4,7-trione derivatives were synthesized by the pharmacophore-hybridization approach. In this study, pyrazolone-fused azanaphthoquinone (or pyrazolone-fused quinoline-5,8-dione) derivatives were synthesized regioselectively through the hetero-Diels-Alder reaction of indazol-3,4,7-trione derivatives with azadiene. In addition, its structure identification and biological activity were investigated.



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Poster Presentation : **ORGN.P-327**

Organic Chemistry

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Design of dispersant for highly stable BaTiO3 slurry systems and robust dielectric sheets

Jung Jin Park, Eun Jung Lee, Yong Park, Jong Ho Lee[*]

MLCC Development Team, Samsung Electro-Mechanics, Korea

To fabricate high-end MLCC with thin dielectric layers, there is a pressing need to develop a technology for the dispersion stability of nanoparticles and the mechanical strength of dielectric sheets. The chemical structures of dispersants are important because they determine the stability of slurry and the failure mode at interfaces of metal-oxide particles and polymeric binders. Here, we characterize the dispersants with several kinds of chemical structures. The thermal, chemical, and mechanical properties of dispersants are differentiated by their structures of functional groups. We establish the design rule of the dispersant structure and apply the dispersant with a new structure. It leads to outstanding dispersion stability, sheet strength, and chemical resistance, which are required to develop ultra-thin dielectric sheets.

Poster Presentation : **ORGN.P-328**
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Efficient and Sustainable Synthesis of Alkenes through Electrochemical Reduction of Alkynes

So Yeun Lim, Hyun-Suk Yeom[1,*], Joon Ho Lee[1,*]

Department of Chemistry, Hanyang University, Korea
[1]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

The alkenes are useful building blocks and have been widely used in pharmaceutical chemistry, and the polymer industry. The transition metal–catalyzed selective semi-hydrogenation of alkynes is the cleanest and most powerful method for the synthesis of cis-olefins. However, this process is often complicated due to using stoichiometric amounts of reducing reagents. Moreover, poor chemo and stereo-selectivity and over-reduction of alkenes to alkanes are observed in most cases. Recently, we have developed an electrochemical semi-hydrogenation method for the synthesis of alkenes from alkynes. This process allows a reduction of the carbon-carbon triple bond using cheap sacrifice metal in methanol without using traditional metal catalysts and reducing agents. Internal- and terminal alkenes are produced quantitively from alkynes without over-reduction, as well as Z-alkenes are predominant. These details will be presented in this presentation.

Poster Presentation : **ORGN.P-329**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Shape-Assisted Self-Assembly of Molecular Pringles

Hongsik Kim, Nam Ki Lee*, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Molecular self-assembly process is guided by the shape of molecules, since the three-dimensional structure of individual molecules dictates how they can interact each other to form larger structures. Conventional strategies for creating well-ordered molecular assemblies utilize hydrogen bonding or van der Waals forces. In this presentation, we will discuss non-planar π-conjugated molecules that readily assemble into columnar stacks. Unlike typical π-conjugation, these molecules adopt a Pringles®-like hyperbolic paraboloid shape with two orthogonal curvatures to support vertical π-stacks without assistance from strong intermolecular interactions. With suitable alkyl chains as solubility controller groups, these molecules rapidly form crystals with extraordinarily large aspect ratios in polar solvents. Kinetic analysis on the real-time crystal growth revealed the impacts of molecular shape and dimensions on the self-assembly behavior. We show that the long linear crystals can function as waveguides, which demonstrates the practical utility of molecular self-assembly by rational structure design.

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Polydopamine-Coated Dielectric Layers for Enhancement of Mechanical Properties

Yong Park, Jung Jin Park, Eun Jung Lee, Jong Ho Lee*

MLCC Green Chip Lab, Samsung Electro-Mechanics, Korea

To fabricate ultra-small and ultra-high capacity of the MLCC, ultra-thin layer and high stacking design of the dielectric sheet are in progress.The higher the ultra-thin dielectric sheet is stacked, the more important the deformation and adhesion are. However, deformation and adhesion have a trade-off relationship, making it difficult to control.To solve this problem, a study was conducted to introduce polydopamine into dielectric sheets.Polydopamine with a catechol group is a universal adhesive material that adheres to an organic or inorganic surface and not only increases adhesion, but also contributes to improving sheet strength through intermolecular bonding.The dielectric slurry to which polydopamine is applied prevents aggregation between particles, thereby increasing dispersibility and strengthening binding force between binders.In conclusion, the dielectric sheet to which polydopamine was applied increased adhesion force and strength.

Poster Presentation : **ORGN.P-331**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Fluoroethers via SN1 -type ring-opening fluorination

Chaeyeon Lee, Sueun Lee, Hee Nam Lim[1,*]

Yeungnam University, Korea

[1] *Department of Chemistry and Biochemistry, Yeungnam University, Korea*

In the poster presentation, we report a new synthetic method of fluoroethers. The developed method used α-substituted coumaranone-oximes and α-aryloxy indanone-oximes as substrates, and diethylaminosulfur trifluoride(DAST) as a dual-role reagent that provides fluoride and activates oxime hydroxyl group. The reaction mechanism is based on SN1-type fluorinative Beckmann fragmentation. Due to mild reaction condition and good chemoselecitivty, various tertiary and secondary fluoroethers were obtained in moderate to high yields.

Poster Presentation : **ORGN.P-332**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Structural Modification of 3D Asymmetric Electron-Blocking Materials for Stable Blue Phosphorescent Organic Light-Emitting Diodes

Eunhye Hwang, Tae-Hyuk Kwon*

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

With the theoretical internal quantum efficiency up to 100%, blue phosphorescent organic light-emitting diodes (PhOLEDs) have been developed as a promising candidate of the next-generation high efficiency OLED displays. For their commercialization, however, there is still a challenge of poor operational stability due to the large band gap and high turn-on voltage requirements of blue emitters, which is resulted in severe decomposition of devices by leakage of charges and triplet excitons into interfacial layers.Herein, to achieve effective triplet confinement and decrease in turn-on voltage of blue PhOLEDs, four types of asymmetric electron-blocking materials (EBMs) are developed based on spatially twisted molecular configurations. The most twisted compound, DBFCz$_2$-Ph, shows the highest thermal stabilities and good energy level alignments for selective carrier transport. Moreover, its molecular orientations are revealed to be face-on-dominated compared to the others owing to the highest dipole moment, which is beneficial for efficient hole transport and reduces the turn-on voltage. As a result, the maximum power efficiency of 33.9 lm W^{-1} of the blue PhOLEDs is achieved by employing DBFCz$_2$-Ph. Furthermore, the operational lifetime of the DBFCz$_2$-Ph-based PhOLEDs is extended up to 21% compared to the reference device using 3,3'-di(9*H*-carbazol-9-yl)-1,1'-biphenyl (mCBP) as a conventional EBM.

Poster Presentation : **ORGN.P-333**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Total Synthesis of Exiguamines

Yee Hwan Kim, Chulbom Lee*

Department of Chemistry, Seoul National University, Korea

Exiguamines are natural products extracted from Neopetrosia exigua by Anderson group in 2006. One of the most important features of this natural products is that they are IDO inhibitors. IDO is an enzyme that can decrease the concentration of tryptophan. This reduces immunity action of T-Cell. Tumor cells overexpress IDO to avoid immunity action and inhibition of IDO might result in antitumor immunity. In this research, we developed novel strategy for total synthesis of Exiguamines. This route requires prefunctionalization of only one fragment and there’s no regioselectivity issue from oxidation step. Furthermore, using this route with chiral adrenaline as substrate can make enantiopure Exiguamine B and its unnatural diastereomer. Our goal is to synthesize Exiguamines and its unnatural isomers and evaluate each biological activities.

Poster Presentation : **ORGN.P-334**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Ir(Ⅲ)-based Dendrimer-Conjugated Sonosensitizer to Overcome Shortages of Photodynamic Therapy

Gwang su Yoon, Tae-Hyuk Kwon*

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

Sonodynamic therapy (SDT) is the newly developed non-invasive cancer treatment method to overcome photodynamic therapy (PDT). PDT is a non-invasive cancer treatment method using light and photosensitizer (PS). However, the light has a low penetration depth problem in tissue (10cm) by transmitting ultrasound, has emerged as the new alternative to PDT. Nevertheless, SDT has the disadvantages of low ROS generation and low biocompatibility of existing sonosensitizer. Recent studies have shown that the higher the quantum yield of sonosensitizer, the higher the ROS generation.Herein, we propose the Ir(Ⅲ)-based sonosensitizer conjugated with dendrimer to overcome the above problems. Our Ir(Ⅲ) complexes have various advantages such as high quantum yield, long lifetime, and high ROS generation. Additionally, we conjugate the dendrimer to Ir(Ⅲ) sonosensitizer for increasing biocompatibility. This Ir(Ⅲ) sensitizer conjugated dendrimer nanoparticle can form a spherical shape dendrimer micelle that can increase the water solubility of the nanoparticle and solve drug leakage problems. In addition, maleic anhydride introduced at the end of the dendrimer is separated from only the acidic cancer environment and converted into an amine, allowing nanoparticles to have a positive surface charge. Therefore, the cancer-targeting ability of these nanoparticles will increase and the therapeutic effect can be maximized.

Poster Presentation : **ORGN.P-335**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of pyrazoline derivatives from [3 + 2] cycloaddition of Nitrile imine with N-silyl enamine

Sooyeon Yun, Seewon Joung[1,*]

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

Enamines showing a variety of applicability for organic synthesis as good nucleophiles, and can be utilized for synthesis of amines,amidines, and other nitrogen containing functional group, showing various application to pharmaceutical chemistry. Our previous studies have focused on the synthesis of cyclic amidines using organic azides with enamine intermediates from the borane-catalyzed hydrosilylation of isoquinolines and quinolines. This study is about construction of pyrazoline ring by using [3 + 2] cycloaddition of the nitrile imine with the N-silyl enamine from the readily available N-heteroarenes.

Poster Presentation : **ORGN.P-336**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Developing Strategies to Utilize Unstable Diazoalkanes from N-Silyl Enamines and Organic Azide

Vinh Do cao, Seewon Joung[1,*]

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

In recent research, we have developed a synthetic strategy to furnish Z-amidines from cyclic N-silyl enamines and organic azides via [3+2] cycloaddition following the rearrangement pathway. Herein, we continued using borane-catalyzed hydrosilylation conditions for conjugated nitriles to obtain linear N-silyl enamines. These linear N-silyl enamines also underwent [3+2] cycloaddition with organic azides, but triazoline intermediate occurred a different rearrangement pathway, which produced E-formamidines and diazoalkanes as co-products. Diazoalkane was an extremely unstable compound, but it was a versatile structure to furnish abandon of functional groups in organic synthesis. Under this observation, we have already developed the new conditions to convert diazoalkanes to ester and pyrazolidines under mild conditions.

Poster Presentation : **ORGN.P-337**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Anion-Induced and Aggregation-Enhanced Light Emission of Dicationic Fluorophores: Molecular-Level Control of Hydrophobicity for Sensitivity and Selectivity

Chungryeol Kim, Dongwhan Lee[*]

Department of Chemistry, Seoul National University, Korea

Weakly coordinating anions have wide applications in catalysis and electrochemistry. To distinguish between different levels of hydrophobicity, general principles and parametrizations are still in need. The difficulty arises from the diminished strength of ionic interactions in the presence of water molecules, making it challenging to quantify hydrophobicity outside the classical Hofmeister series in aqueous environments. We have developed dicationic fluorophores to differentiate hydrophobic anions in water by aggregation-induced emission. Depending on the chemical structure, distinct emission response profiles were observed, and the underlying structure–property relationship was investigated by X-ray structure and Hirshfeld surface analyses. We found that the sensitivity and selectivity of the fluorophores towards specific anions can be tailored by varying the peripheral alkyl chains around the common dicationic polyheterocyclic core. In this presentation will be discussed the key design principles, synthetic implementations, and practical applications of designer molecular cations to detect and differentiate hydrophobic anions in water.

Poster Presentation : **ORGN.P-338**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Azepane-Derived β-Amino Acid as a New Helix-Forming Unnatural β-Peptide Building Block

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

The ability of cyclic ring-constrained β-amino acids to adopt various characteristic folding patterns with relatively rigid conformation makes them useful building blocks for β-peptides. As heterocyclic ring moieties are abundant in many natural products with significant biological functions, N-fused heterocyclic β-amino acids have received some attention for decades. In addition to their conformational stability, their ability to introduce several functional groups via N-functionalization makes N-fused heterocyclic β-amino acids as promising building blocks for helical peptides.1 We have recently shown the ability of cis-4-aminopiperidine-3-carboxylic acid (cis-APIC) as a 11/9- or 12/10- mixed β-peptides building block.2 However, N-fused heterocyclic β-amino acids with seven-membered ring is rarely studied. Herein, we synthesized enantiopure azepane derived β-amino acid (4S,5R)-5-aminoazepane-4-carboxylic acid (cis-AAZpC) with our efficient synthetic pathway involving acid-catalyzed ring expansion of N-Boc-4-piperdone followed by solvent-free reductive amination. Furthermore, we synthesized several 12/10-helical β-peptides and characterized their conformation using circular dichroism and single crystal X-ray diffraction analysis. We assessed the efficacy of cis-AAZpC as a promising building block for producing well-organized helical peptides.

Poster Presentation : **ORGN.P-339**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Rational design of nitrogen-doped carbon encapsulated Ni catalyst for efficient reduction of nitroarenes in the continuous flow system

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As Ni catalyst Ni@N-C newly developed by controlled pyrolysis of adenine and NiCl2·6H2O mixture with convenient, facile, efficient, and selective reduction of nitro-containing arenes and heteroarenes were promoted in 5 min at room temperature utilizing inexpensive NaBH4 as the hydrogen source. A wide variety of nitro derivatives, including pharmaceutical molecules, were successfully reduced to corresponding amines in excellent yields, catalyzed by Ni@N-C in general batch conditions. The reactivity and selectivity of nitro reduction were further enhanced by continuously flow reaction, especially in a new-designed Y-type column, and long-term experiment was tested for 24h producing Osimertinib intermediate in gram scale without any nickel metal contamination and silica gel chromatography purification, indicating a green technology in organic synthesis.

Poster Presentation : **ORGN.P-340**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Photoinduced Transition-Metal-Free Chan–Evans–Lam-Type Coupling: Dual Photoexcitation Mode with Halide Anion Effect

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In this article, we describe a photoinduced method for the transition-metal-free formation of C(aryl)-N bonds between 2,4,6-tri(aryl)boroxines or arylboronic acids and 1,4,2-dioxazol-5-ones (dioxazolones) as the amide coupling partner. The addition of chloride anion, either by photodissociation of chlorinated solvents or as a separate additive, was found to play a crucial cooperative role, enabling the formation of a diverse range of synthetically versatile N-arylamides under mild photo conditions. This transition-metal-free Chan-Evans-Lam-type coupling was demonstrated by large-scale reactions, synthesis of ^{15}N-labeled arylamides, and its applicability to biologically relevant compounds. Mechanistic investigations revealed two distinctive photoexcitations involved in the process, with the first excitation leading to the transition-metal-free activation of dioxazolones through single electron transfer (SET) facilitated by the chloro-boron adduct. The second excitation enabled the otherwise-inoperative 1,2-aryl migration of the N-chloroamido-borate adduct.

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Poster Presentation : **ORGN.P-341**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Tube-Like Peptoid Structures

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Peptoids, N-substituted glycine oligomers, are known to be fascinating peptidomimetics that have a plenty of advantages including higher cellular permeability, improved proteolytic stability, and ease introduction of structural diversity. Additionally, various peptoid derivatives which could be utilized as chemical tools for protein-protein interaction (PPI) inhibition, drug delivery and antimicrobial function have been developed. In addition to our efforts to the development of cyclic and complex peptoid structures, we envisioned to synthesize tube-like peptoid structures which should be structurally challenging and possess interesting chemical/physical properties.At first, tube-like peptoid structures which were composed of two identical cyclic peptoids connected by two tethers were designed. Double-stranded peptoids which were tethered by ethylene glycol bis(3-aminopropyl) ether were synthesized on solid-phase. Then, each strand was successfully macrolactamized. However, crossed dual macrolactamized products were also detected in small amounts to give bicyclic peptoids. These structures should be also unique and interesting. Second cyclization was carried out by ring-closing metathesis or disulfide-bond formation to afford desired tube-like peptoid structures. The final products were purified and analyzed by HPLC and MALDI-TOF spectrum, but further optimization is in progress.

Poster Presentation : **ORGN.P-342**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Chain Walking as a Strategy for Iridium-Catalyzed Migratory Amidation ofAlkenyl Alcohols to Access α-Amino Ketones

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While an accessing valuable nitrogen-containing compounds is an appealing field in organic chemistry, catalytic carbon—nitrogen bond formation of hydrocarbons is a fascinating synthetic tool. Although a number of approaches to generate an α-amino carbonyl scaffold have been developed well, however, functionalization at remote and unfunctionalized aliphatic sites installing an amino group remains underdeveloped. Herein, we introduce the tandem iridium catalyzed redox-relay amidation of alkenyl alcohols via chain walking and metal-nitrenoid transfer, which eventually offers a new synthetic route to various α-amino ketones with excellent regioselectivity. Experimental result that unrefined isomeric mixture of alkenyl alcohols can be utilized as available starting materials in this system giving the additional virtue in synthetic utility, giving the regioconvergent amidated ketones. Detailed tandem process involving two key components of redox-relay chain walking and intermolecular nitrenoid transfer assisted by hydrogen bonding was proposed via mechanistic experiment and density-functional theory (DFT) calculation, thus representing the competence of Ir catalysis for the olefin migratory C—N coupling with high efficiency and exquisite selectivity.

Poster Presentation : **ORGN.P-343**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Total Synthesis of a Duocarmycin Analogue Including a Chiral Indoline via an HFIP-Induced Intramolecular Friedel-Crafts Alkylation

Eunseok Choi, Kyungmin Yun, Eunwoo Baek, Geonhui Ko, Sang Jeon Chung[1,*]

Biopharmaceutical Convergence, Sungkyunkwan University, Korea
[1]*College of Pharmacy, SungKyunKwan University, Korea*

Duocarmycins are a class of cytotoxic compounds with a potent anticancer effect but also severe hepatotoxicity and have been investigated as potential candidates for use in antibody-drug conjugates (ADCs). Currently, more than 15 duocarmycin-based ADCs have been studied preclinically, and some of them such as SYD985 have been granted Fast-Track Designation status by the FDA. Therefore, investigating methods for a scalable, effective, and facile synthesis of duocarmycin is essential. Originally, the indoline of the DNA alkylating unit was synthesized via transmetalation, followed by ring opening of a chiral epoxide. The main drawbacks of the conventional method were high moisture sensitivity and low yield (

Poster Presentation : **ORGN.P-344**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of SO218F-functionalized PET radiotracers through drug repurposing

<u>Jaegwan Kim</u>, Min Ho Jeon, Joong-Hyun Chun*

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The development of an efficient method for incorporating 18F into radiotracers is required for successful positron emission tomography (PET) imaging. Recently, the use of sulfur(VI) fluoride exchange (SuFEx) chemistry to exploit fluorosulfuryl functional scaffolds has attracted significant attention as a versatile chemical arsenal pharmaceutical and material science. In the present study, we report a radiofluorination method that involves the direct use of a QMA-eluted [18F]fluoride source to functionalize sulfur-heteroatom frameworks. Various drug-relevant precursors were radiolabeled with cyclotron-produced 18F ions with moderate-to-good radiochemical conversion (~88%). Although phenolic substrates can be directly converted into the corresponding aryl [18F]fluorosulfate, aqueous isotopic exchange proved to be an expedient approach for a variety of sulfur–oxygen skeletons. In addition, the isotopic 18F-activation of sulfur–nitrogen scaffolds was an efficient route for the production of drug-relevant sulfamoyl [18F]fluorides. This labeling protocol represents an efficient route for incorporating 18F into sulfur–oxygen and sulfur–nitrogen frameworks, facilitating rapid radiochemistry screening. The application of this approach to drug-relevant compounds also enables the expedient evaluation of new 18F-functionalized SuFEx radiotracers for potential PET applications. This work was supported by NRF (NRF-2022R1A2C2004064).

Poster Presentation : **ORGN.P-345**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Blending Low-Frequency Vibrations and Push-pull Effects Affords Superior Photoacoustic Imaging Agents

Le Yu, Jusung An, Ji Hyeon Kim, Jaewon Kim, Jungryun Kim, Hyeonji Rha, Jieun Lee, Qihang Ding, Injun Lee, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Photoacoustic imaging (PAI), a state-of-the-art noninvasive in vivo imaging technique, has been widely used in clinical disease diagnosis. However, the design of high-performance PAI agents with three key characteristics, i.e., near-infrared (NIR) absorption (λabs > 800 nm), intense PA signals, and excellent photostability, remains a challenging goal. Herein, we present a facile but effective approach for engineering PAI agents by amplifying intramolecular low-frequency vibrations and enhancing the push-pull effect. As a demonstration of this blended approach, we constructed a PAI agent (BDP1-NEt2) based on the boron-dipyrromethene (BODIPY) scaffold. Compared with indocyanine green (ICG, an FDA-approved organic dye widely utilized in PAI studies; λabs = 788 nm), BDP1-NEt2 exhibited a UV-Vis-NIR spectrum peaked at 825 nm, superior in vivo PA signal intensity and outstanding stability to offer improved tumor diagnostics. We believe that this work provides a promising strategy for chemists to develop the next generation of PAI agent.

Poster Presentation : **ORGN.P-346**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Total Synthesis of Madeirolide A

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Madeirolide A, isolated from a marine sponge Leiodermatium species by Wright and Winder in 2009. It has been reported that its inhibitory activity against Candida albicans is significant 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 madeirolaide A, including our own, have been reported. However, a complete total synthesis of madeirolide A has not been reported yet, and the absolute stereostructure and bioactivity of the natural product remains to be explored. We propose the construction of madeiorlide A through fragment-assembly of absolutely stereo-controlled A-C subunits, thus maximizing stereochemical flexibility. Constructions of three oxacycles have been carried out through visible-light-induced radical cyclization.

Poster Presentation : **ORGN.P-347**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Fluoride and Chloride Salt Extraction by a Pyrrole-Strapped Calix[4]pyrrole

Nam Jung Heo

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Diphenylpyrrole-strapped calix[4]pyrroles 1 have been synthesized and their anion binding features were investigated by means of ^1H NMR spectroscopy and single crystal X-ray diffraction analyses. In addition, receptor 1 is able to extract the hydrophilic fluoride anion (as both its TEA^+ and TBA^+ salts) as well as the chloride anion into a $CDCl_3$ phase from an aqueous solution. Cation metathesis using TBAI and the use of dual host system involving crown ethers enables receptor 1 to extract alkali metal fluoride or chloride salts with high efficiency from water.

Poster Presentation : **ORGN.P-348**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Calix[4]pyrrole biscrowns having a deep cavity: synthesis and ion binding properties

Juho Yang

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A series of doubly strapped calix[4]pyrroles 2-4 with different sizes of crown ethers have been synthesized by the reaction of the meso-tetra-4-hydroxyphenyl-calix[4]pyrrole (5) with tri-, tetra-, and penta-ethylene glycol ditosylates, respectively, in the presence of K_2CO_3 as a base. Calix[4]pyrrole biscrowns 2-4 proved capable of selectively binding the fluoride and the bicarbonate anion among the test anions in $CDCl_3$. By contrast, calix[4]pyrrole biscrown-5 and -6 (3 and 4) were found to bind only the sodium cation (Na^+) among the alkali metal cations (as their perchlorate salt forms) while receptor 2 with relatively small crown ether had no affinity for those cations in 10% methanol-d_4 in $CDCl_3$. It was also revealed via ^{1}H NMR spectroscopic analyses that receptors 2 and 3 complex CsF and CsCl with high selectivity over other alkali metal fluoride and chloride salts but with different binding modes. For instance, receptor 2 complexed the cesium cation with the π-electron-rich calix[4]pyrrole cavity with the fluoride or the chloride anion hydrogen bonded to the four calix[4]pyrrole NHs while receptor 3 bound the cesium cation via either of its two crown-5 rings.

Poster Presentation : **ORGN.P-349**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Environmentally Sensitive Two-Photon Fluorescence Probe For Biomedical Applicantions

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There are various environments within the cell. Local environmental parameters such as polarity, pH, viscosity, and temperature regulate intermolecular interactions and affect the stability of the microenvironment in cells. Therefore, it is necessary to monitor local environmental parameters. Especially, viscosity plays a role in maintaining signal transmission, transportation and diffusion of substances, and cell metabolism. Abnormal viscosity causes various diseases such as cardiovascular disease, diabetes, Alzheimer's disease, and high blood pressure. Therefore, it is important to monitor changes of viscosity to diagnose related diseases.Fluorescent environment-sensitive probes are known to have high sensitivity and high spatial and temporal resolution. Thus, we synthesized many fluorescent probes and tested probes in viscosity environment made with glycerol or poly(ethylene glycol). We observed the fluorescence intensity of the probe increased as viscosity of solvent increased. Since our probes are environmentally sensitive, they are expected to be used to observe changes in intracellular viscosity and diagnose viscosity related disease. Furthermore, we will show the application of our probes to live cell.

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Poster Presentation : **ORGN.P-350**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a Two-Photon Red Emissive Dye for Senescence-Associated Beta-Galactosidase (SA-gal) Studies

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Two-photon red emissive dyes have emerged as promising tools for fluorescence imaging with improved spatial resolution and depth penetration in thick samples. Here, we describe the development of a red emissive dye with high quantum yield under aqueous conditions and improved one and two photon properties. This dye emits bright fluorescence in various cell lines, including HeLa, SKOV-3, and OVCAR-3. We also attached a galactosidase receptor to the dye, which resulted in diminished fluorescence. However, the fluorescence could be restored in the presence of beta-galactosidase enzyme. In vitro studies showed that the dye reacted quickly to the enzyme and worked under various pH conditions. These properties make it a useful tool for studying senescence-associated beta-galactosidase (SA-gal) in cells and senescence models, which are important in understanding the aging process and related diseases.

Poster Presentation : **ORGN.P-351**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Enantioenriched Cyclic Allene Precursors Using Recyclable Chiral Auxiliaries

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[1]Department of Chemistry, Ajou University, Korea

This study aims to prepare various enantioenriched cyclic allene precursors, which have recently gained attention as highly reactive coupling agents for the rapid synthesis of cyclic complex molecules. Cyclic allenes are unstable molecules that typically exist in the form of metal complexes or can only be indirectly isolated through trapping due to the ring distortion strain. The current best method for obtaining enantiomerically pure cyclic allenes involves chiral separation of racemic cyclic allene precursors using expensive supercritical fluid chromatography (SFC) equipped with preparative chiral columns. However, no reported method exists for the synthesis of enantiopure cyclic allenes without the support of chiral SFC technique. In this study, we developed a synthetic route toward enantioenriched cyclic allene precursors utilizing recyclable chiral auxiliaries, (S)- and (R)-1-amino-2-methoxymethylpyrrolidines (SAMP and RAMP respectively). This synthetic method is believed to significantly reduce the barrier to preparing enantioenriched cyclic allene precursors, which are useful building blocks for asymmetric transformation.

Poster Presentation : **ORGN.P-352**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Cancer-targeted two-photon photosensitizer : small-molecule strategy

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

Two-photon excitation (TPE) has been used as an important tool for bioimaging and has great potential for use in photodynamic therapy. However, this technique requires an efficient photosensitizer, and a simple and flexible strategy for developing two-photon photosensitizers. Here we propose a selenium-containing small-molecule two-photon photosensitizer (BSe). Compared with dyes containing BSe and various heteroatoms (NH, O, S, Te), the photophysical properties and ROS generating ability were investigated. BSe showed excellent ability to generate type I-based ROS induced by 730 nm two-photon excitation and low cancer toxicity. In addition, it can exert a function as a photosensitizer even under hypoxic conditions. BSe is also easily modified into a cancer-targeted agent, BSe-B. By applying BSe-B to 3D-spheroids and colorectal-cancer patient-derived samples, its potential to exert photodynamic therapy towards cancer cells was demonstrated in a site-specific manner. This result will provide an efficient tool for developing two-photon photosensitizers.

Poster Presentation : **ORGN.P-353**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Indolocarbazole-Pyridinium Foldamers with Internal Tubular Cavities for Accomodating Multiple Halide Ions

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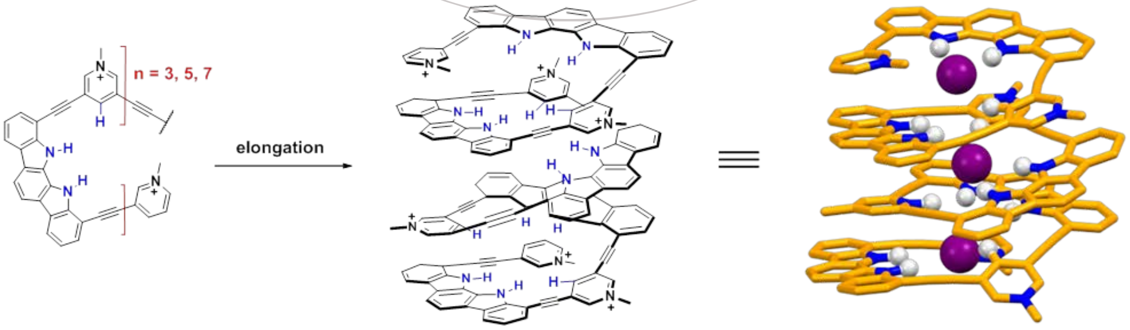
A series of indolocarbazole-pyridinium oligomers were prepared by connecting two repeating aryl units through ethynyl bonds in an alternative way. The oligomers fold into helical structures with generating an internal tubular cavity wherein all the hydrogen bonding donors of indolocabazole NHs and pyridinium p-CHs are oriented for binding halide ions. The number of the bound halide ions in the internal cavity depends on the length of foldamers. It is quite rare to accommodate multiple halide ions in the single-strand helical foldamer although some examples of double- and triple-strand foldamers are known. This is because single-strand helices may be easily ruptured by repulsive interaction between the bound anions, compared with mechanically intertwined double and triple helices. Details including syntheses and structural analyses will be discussed in the poster presentation.



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Organic Chemistry

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A fluorescent probe for selective monitoring of COX-2 in intervertebral disc cells and tissues

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Intervertebral disc (IVD) degeneration is one of the serious health problems that people complain of these days. In a recent study, the expression of cyclooxygenase-2 (COX-2) increased with the degree of IVD degeneration. Based on this, we developed a fluorescent probe for targeting COX-2, indomethacin-adopted benzothiazole-pyranocarbazole (IBPC1), to effectively observation of IVD degeneration. The fluorescence intensity of IBPC1 increased with COX-2 expression level by inflammatory stimuli in nucleus pulposus cells (NPCs) and IVD degeneration model rat tissues. These results demonstrate that IBPC1 can clearly distinguish the COX-2 expression level according to the induction of inflammation in cells and IVD degeneration model rat tissues.

Poster Presentation : **ORGN.P-355**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Endo-Selective Intramolecular Alkyne Hydroamidation Enabled by NiH Catalysis Incorporating Alkenylnickel Isomerization

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Intramolecular hydroamidation of alkynes is a valuable synthetic transformation leading to synthetically valuable cyclic enamides. One of the main challenges in this process is to attain precise regioselectivity, especially for *endo* cyclization that leads to six-membered and larger azacyclic rings. Herein, we report a NiH-catalyzed intramolecular hydroamidation of alkynyl dioxazolones that allows regioselective access to a range of six- to eight-membered endocyclic enamides, thus granting ring sizes and selectivity that were beyond reach with the previous strategies. Comprehensive experimental and computational investigations suggested that Ni(I) catalysis is operative in the current process, proceeding via regioselective syn-hydronickelation, alkenylnickel *E*/*Z* isomerization, and Ni-centered inner-sphere nitrenoid transfer. In particular, the key alkenylnickel isomerization step, which previously lacked mechanistic understanding, was found to take place through the η2-vinyl transition state. The obtained endo selectivity was proven beneficial in terms of synthetic virtues, as the versatile enamide functionality within the rings could be subsequently harnessed for a number of diastereoselective transformations to lead to highly functionalized δ-lactam scaffolds.

Poster Presentation : **ORGN.P-356**

Organic Chemistry

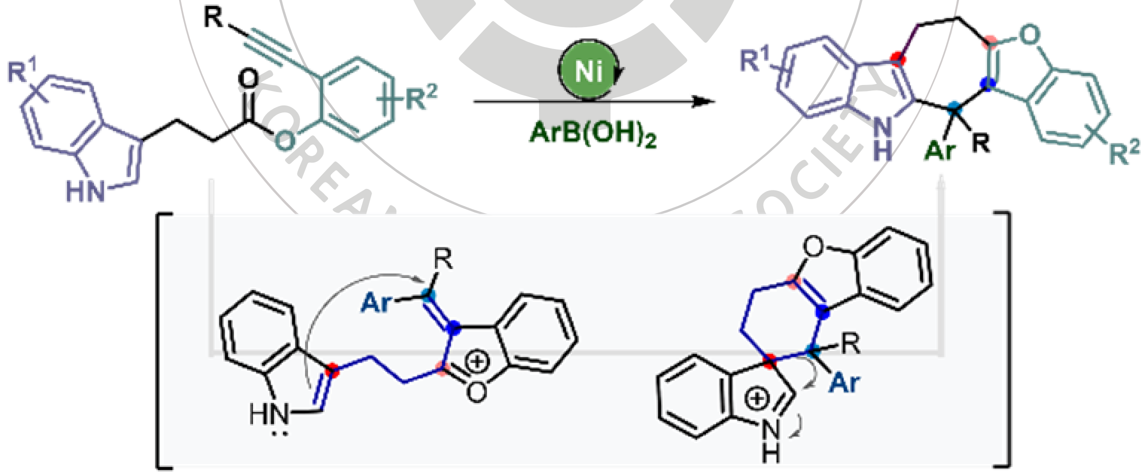
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Construction of a Pentacyclic Framework Enabled by Nickel Catalysis

Jaehan Bae, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

We present a novel nickel-catalyzed reaction of indole-tethered 2-alkynylphenol esters with various (hetero)aryl boronic acids, resulting in the synthesis of diversely functionalized pentacyclic benzofurocyclohepta[b]indole derivatives. This un-precedented cascade reaction involves the arylative cyclization of alkynes, nucleophilic attack of the indole moiety on the oxonium ion intermediate, 1,2-alkyl group migration, and aromatization. The synthesized molecules exhibit exceptional cytotoxicity against multiple cancer cell lines while maintaining biocompatibility towards healthy cells.



Ni-catalyzed functionalization & cascade ring construction

Poster Presentation : **ORGN.P-357**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Multidimensional ligand modulation of rhodium catalysts for selective intra- and intermolecular C–H amidations

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Department of Chemistry, KAIST, Korea

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We report herein a series of tailored $Cp^{X}Rh(LX)Cl$ catalyst systems for the outer-sphere C–H amidations discovered by high-throughput experimentation. By employing diverse sets of Cp-tunable group 9 $[Cp^{X}MCl_2]_2$ precatalysts in combination with bidentate LX-type ligands, we have established a premixing protocol for the rapid and convenient *in situ* generations of an array of half-sandwich metal complexes. Benefited from the multidimensional approach to simultaneously screen the metal center, Cp^{X}, LX-type ligands, and nitrene precursors, optimal $Cp^{X}Rh(III)(LX)$ catalysts were quickly identified for intra- and intermolecular C–H amidations, and also for an enantioselective transformation by using *N*-tosyloxycarbamates as the nitrenoid precursor.

Poster Presentation : **ORGN.P-358**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ruthenium-Catalyzed Three-Component Deaminative Coupling of Phenols with Aldehydes and Enamines

Donghun Hwang, Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Multicomponent coupling reactions are an efficient and versatile tool for synthesizing complex molecules in a single step. They provide access to diverse molecules that are difficult to prepare with traditional methods and have a high atom economy. It can also serve as a key step in developing new synthetic strategies, making them an important area of research in modern organic chemistry. In 2021, the Yi and our group reported a mild and efficient dehydrative coupling between phenols and aldehydes catalyzed by the tetranuclear Ru–H complex, and 3,4,5,6-tetrachloro-1,2-benzoquinone to synthesize xanthene derivatives.1 Inspired from this result, we designed an elaborate three-component coupling between phenols, aldehydes, and enamines via C–H activation and deaminative coupling in the same catalytic platform. The incorporation of enamine substrates further expanded the scope of products, enabling us to produce C9-functionalized xanthenes in a selective manner. This strategy represents a promising approach for the synthesis of heterocyclic compounds and we plan to further explore its potential for the synthesis of a more complicated heterocyclic system with variations in reagents.

Poster Presentation : **ORGN.P-359**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Selective detection of Homocysteine in aqueous buffered solution and 10% Human serum by peptide-based fluorescent ensemble system using amino terminal copper and nickel (ATCUN) motifs

Sujin Lee, Keun Hyeung Lee[1,*]

Department of Chemistry and Chemical Engineering, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

According to clinical studies, an increase in total homocysteine (Hcy) concentration in the blood is related to coronary artery disease, stroke, and osteoporotic fractures. Therefore, there is a high demand for the development of Hcy sensing probes in blood. For this, a peptide-based fluorescent ensemble system using amino terminal copper and nickel (ATCUN) motif was designed to detect Hcy in aqueous solutions as well as serum. ATCUN binding motif has been used as an ensemble system with Cu(II) (probe-Cu2+) because the binding motif (Xaa-Zaa-His) had a potent binding affinity for Cu(II) that fully quench fluorophore of ATCUN binding motif. We synthesized fluorescent labeled peptides corresponding to ATCUN binding motif using 4-Nitro-2,1,3-benzoxadiazole (NBD) fluorophores with visible light excitation. Fluorescent ensemble consisting of NBD labelled tripeptide (NBD- Xaa-Zaa-His) and Cu(II) showed both fluorescence and absorbance changes to biothiols in aqueous solutions. Specially, ensemble system based on tripeptide consisting of SerDapHis provide selective and sensitive turn-on detection of Hcy among biothiols. NBD labeled tripeptide (NBD-SerDapHis) formed the ensemble with Cu2+ for a fluorescent detection for Hcy. The addition of Hcy promptly took Cu2+ from the ensemble in buffered aqueous solutions, causing a turn-on fluorescent response. The ensemble sensitively detected the low concentration of Hcy ranged from 10 μM to 100 μM in aqueous solutions and 10% human serum. The detection limit measured to be 174.8 nm in aqueous buffer solution and 287.2 nm in 10% human serum. In this feature article, we will further design a fluorescent ensemble system with Cu(II) for ratiometric detection of Hcy in human serum using FRET based ensemble.

Poster Presentation : **ORGN.P-360**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Metal-ATCUN derivative for selective detection of homocystenine among thiols (cysteine and glutathione) in 100% aqueous buffer solution and human serum.

Sumita Subedi, Keun Hyeung Lee[1,*], Inae Jeon

Department of chemistry and chemical engineering, Inha University, Korea
[1]*Department of Chemistry and chemical engineering, Inha University, Korea*

We had synthesized a Fluorescence ensemble sensors (system) based on dansyl labelled peptides to mimic amino terminal copper and nickel binding site (ATCUN) for selective turn-on detection of Homocystenine among biothiols in aqueous buffered solution at physiological pH and human serum. Dansyl fluorophore attached with tripeptide DapDapH shows high binding affinity towards Cu2+ forming 1:1 complex ensemble accompanied by decreasing in fluorescence intensity due to quenching caused by paramagnetic Cu2+. This peptide based ensemble system (Dan-DapDapH) selectively and sensitively detects homocystiene among biothiols like cysteine and glutathione giving turn-on response. Due to high affinity of Cu2+ and thiols when homocystenine is added to peptide based ensemble system (Dan-DapDapH) Cu2+ is removed from the ensemble system hence the quenching is relieved and there is increase in fluorescence intensity.A possible mechanism for this homocystenine-specific selective detection involve the calculation of free sulfur available during the course of reaction whereas no free sulfur detected by DTNB assay for cysteine and glutathione. Oxidation of cysteine and glutathione leave no free sulfur to make complexation with copper so there was no recovery of fluorescence intensity. About 100 μM of homocystenine was enough to completely remove Cu2+ from the peptide based ensemble system (Dan-DapDapH). This peptide based ensemble system (Dan-DapDapH) was successfully applied for selective detection of homocystiene in 10% human serum also. The detection limit measured to be 6.4 nm in aqueous buffer solution and 133 nm in 10% human serum. This is the first reported fluorescent probe to selectively detect homocystiene from cysteine and glutathione based on peptide based ensemble system

Poster Presentation : **ORGN.P-361**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Albumin-mediated “Unlocking” of supramolecular prodrug-like nanozymes toward selective imaging-guided phototherapy

Hee Jeong Kim, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Construction of an activatable photosensitizer and integration into an adaptive nanozyme during phototherapy without producing off-target toxicity remains a challenge. Herein, we have fabricated a prodrug-like supramolecular nanozyme based on a metallic-curcumin and cyanine co-assembly. The albumin-mediated phenol AOH group transformation of nanozyme changes its adjustable oxygen stress from negative superoxide dismutase-like activity of ROS-scavenging to positive photo oxidase activity with an ROS-amplifying capacity. It further increases the depth penetration of a nanozyme in a tumor spheroid, selectively targeting tumorous phototherapy. It also triggers a signal in targeted tumor cells and helps increase cancer cell ablation. This work suggests new options for development of activatable supramolecular nanozymes and provides a synergetic prodrug-like nanozyme strategy for early diagnosis and preclinical phototherapeutics.

Poster Presentation : **ORGN.P-362**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A Novel Synthetic Approach to Xanthones via Cu(II)-Catalyzed Dehydrogenative Conjugate Addition/Aromatization Sequence of Cyclohexyl(2-hydroxyphenyl)methanones

Yoon hu Jang, Nam-Jung Kim[1,*]

College of Pharmacy, Kyung Hee University, Korea
[1]*College of pharmacy, Kyung Hee University, Korea*

Xanthones are kinds of heterocyclic aromatic compounds that consist of γ–pyrone backbone with symmetrically fused two aromatic rings, isolated from various natural sources and medicinal plants and their synthetic analogues. Some of their derivatives have been known to show diverse biological activities such as anticancer, anti-hypertensive, anti-inflammatory effects. Up to date, most of synthetic xanthones are often generated through Friedel-Crafts acylation between oxygenatd arenes and aryl carboxylic acid derivatives, followed by intramolecular nucleophilic aromatic substitution, or the formation of C-O bond between aryl halides and phenols, followed by further cyclization, to the xanthone core framework. However, a novel approach, not following these types of sequences have been rarely studied. Herein, we develop a direct route to xanthones from cyclohexyl(2-hydroxyphenyl)methanone via Cu(II)-catalyzed dehydrogenative chemistry: conjugate addition and following aromatization in a one-step. This methods affords a novel approach to the privileged xanthone scaffold, with a wide substrate scope (a total of 28 compounds, up to 96% yield) in a highly atom-economic manner which doesn't need leaving group atom such as aromatic substitution reaction.

Poster Presentation : **ORGN.P-363**

Organic Chemistry

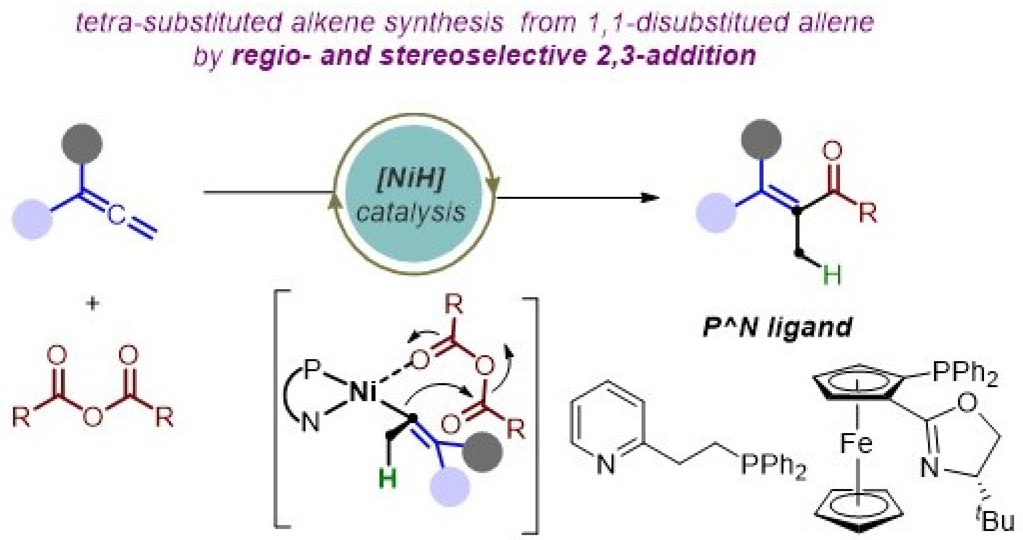
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Base-Free NiH-Catalyzed Regio- and Stereo- selective Hydroacylation of Allenes: A New Route to Synthesis of *Tetra*-Substituted Olefins

Shrikant Tambe, Eun Jin Cho[1,*]

Department of chemistry,Chung-ang university, Chung-Ang University, India
[1]*Department of Chemistry, Chung-Ang University, Korea*

The synthesis of all-carbon tetra-substituted olefins still constitutes a formidable synthetic challenge due to unavoidable issues, including uncontrolled *E/Z* selectivity. Herein, we report a regio- and stereoselective synthesis of *tetra* -substituted olefins via Ni-catalyzed hydroacylation of 1,1-disubstituted allenes with a diverse range of aliphatic and aromatic anhydrides. NiH catalysis mainly with N^N or N^N^N ligand systems had been utilized for bifunctionalization of various alkenes, but not suitable for allenes. In this work, the unprecedented P^N ligand tailored NiH catalysis of allenes in the absence of a base additive has been developed, which shows the opposite regioselectivity to Cu chemistry. The coordination of the extra carbonyl in the anhydride coupling partner to the Ni center makes the challenging intermolecular process more feasible. The chemistry is supported by combined experimental and computational mechanistic studies. The developed method succeeds for both 1,1-disubstituted symmetrical and unsymmetrical allenes, including diaryl allenes, which have been less studied with transitio-n metal catalyzed functionalizations. Furthermore, the synthetic utility of this protocol is demonstrated by the lat-e stage functionalization of estrone-based allene.


tetra-substituted alkene synthesis from 1,1-disubstitued allene
by regio- and stereoselective 2,3-addition
[NiH]
catalysis
+
R
O
R
P
Ni
N
H
P^N ligand
PPh2
Fe
N
tBu

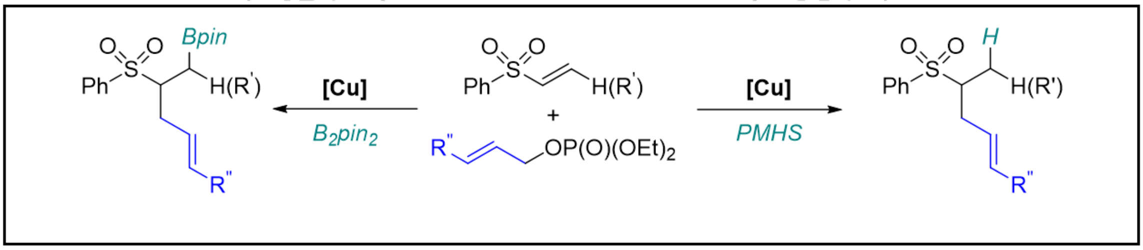
Poster Presentation : **ORGN.P-364**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ligand-Free Boroallylation and Hydroallylation of α,β-Unsaturated Sulfones

Minsoo Lim, Dohyun Park, Jaesook Yun[*]

Department of Chemistry, Sungkyunkwan University, Korea

Sulfone is recognized as the bioisostere of carbonyl groups as it forms a strong hydrogen bond with the target molecules in vivo. For this reason, synthetic functionalization of sulfones with reactive carbon sites drow significant attention in chemical synthesis and medicinal chemistry. We investigated a copper-catalyzed difunctionalization of α,β-unsaturated sulfones under two different catalytic systems (Cu—B and Cu—H), using bis(pinacolato) diboron (B2pin2) or polymethylhydrosiloxane (PMHS), followed by electrophilic trapping of allyl phosphates to access difunctionalized sulfones. The Cu—B catalyzed tandem reaction proceeded in highly diastereoselective fashion to give a single diastereomeric boroallylation product.



Poster Presentation : **ORGN.P-365**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Copper-Catalyzed 1,6-Addition of gem-Diborylalkanes to para-Quinone Methides

He Jing, Meng Deyuan, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

We reported a ligand-free copper-catalyzed 1,6-addition of α-borylalkyl copper species, catalytically generated from gem-diborylalkanes to para-quinone methides. This reaction proceeds with good yield for a variety of para-quinone methides and substituted gem-diborylalkanes with a catalytic amount of CuI as catalyst. The catalytic system provides a cost-effective process with good functional group tolerance under mild conditions.

Poster Presentation : **ORGN.P-366**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Intramolecular Benzyne Cycloadditions using 3-Aminobenzyne Precursors Triggered via 1,3-Aza-Brook-Rearrangement

Ye-Jin Kong, Yong-Ju Kwon, Won-SuK Kim[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Aza-Brook rearrangement has been investigated as a method for the formation of carbon-carbon and carbon-heteroatom bonds in organic chemistry. This rearrangement involves an intramolecular anionic transfer of a silyl group from a carbon to a nitrogen via a hypervalent silicon intermediate. However, there have been few reports on aza-Brook rearrangement due to the relative lack of well-designed amine precursors and the thermodynamic driving force of the weaker N-Si Bond compared to the O-Si bond. Recently, we reported novel 3-amino-2-(tert-butyldimethylsilyl)phenyl triflates as aminobenzyne precursors. A base-mediated 1,3-aza-Brook rearrangement occurred on the aryl group, forming aminobenzyne intermediates, resulting in various aniline derivatives. The application of aza-Brook rearrangement for benzyne formation is noteworthy because it allows control of the timing of benzyne formation. As part of our ongoing efforts in uniting aza-Brook rearrangement with benzyne chemistry, we have focused on the intramolecular benzyne cycloaddition for the synthesis of benzofused N-heterocycles. Herein, we show that the possibility of the synthesis of benzofused N-heterocycles by performing intramolecular [4+2] cycloadditions, ene reactions, and HDDA reactions with a benzyne intermediate formed via 1,3-aza-Brook rearrangement, respectively.

Poster Presentation : **ORGN.P-367**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Continuous Flow Synthesis of cis-Diamino Enones Employing Tandem Relay Cu/Rh Dual Catalysis

Min-Jung Lee, Yong-Ju Kwon, Won-SuK Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The copper-catalyzed azide–alkyne cycloaddition (CuAAC) reaction for the highly regioselective synthesis of N-sulfonyl-1,2,3-triazoles has received significant attention due to their structural potential. Due to the electron-deficient sulfonyl group in N-sulfonyl triazoles, they decompose effectively in the presence of a suitable metal catalyst to produce highly reactive azavinyl carbene. Accordingly, progress has been made in the use of N-sulfonyl triazole as an azavinyl carbine precursor in reactions for a wide range of heterocycles and other scaffolds. Despite the benefits involved, the continuous flow synthesis of N-sulfonyl triazoles has not been reported. In general, the CuAAC reactions for N-sulfonyl triazoles and the decomposition reaction for transition-metal-carbene complexes are highly exothermic reactions. Thus, flow processing would be a versatile tool for the synthesis of them. With these considerations, herein we report the first continuous flow synthesis of N-sulfonyl-1,2,3-triazoles, and the first continuous synthesis of cis-diamino enones employing tandem relay Cu/Rh dual catalysis.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-368**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nickel-Catalyzed Hydroboration of Terminal alkynes to Vinylboronate esters

SeoYeong Jeong, Jeong Woo Lee, Sung You Hong[*]

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

Hydroboration of terminal alkynes has been well-recognized to proceed to access vinylboronate esters. However, hydroboration has not been well developed for terminal alkyl alkynes with a range of functional groups. Herein, we report a catalytic hydroboration of terminal alkynes bearing alkyl, aryl, and silyl moieties via nickel catalytic system under mild reaction conditions. This reaction is tolerant to various functional groups. Mechanistic studies support that involvement of Ni-H complex which is a key intermediate to form vinylboronate esters.

Poster Presentation : **ORGN.P-369**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Radical entry to multi-functionalized quinolines via ATRA-enabled [5 + 1] annulation of 2-alkynylanilines with $CFBr_3$.

Taehyun Oh, Chulbom Lee[1,*], Eun Jin Cho[2,*]

Department of Chemistry, Seoul National University, Korea
[1]Division of Chemistry, Seoul National University, Korea
[2]Department of Chemistry, Chung-Ang University, Korea

The synthesis of 4-bromo-2-fluoroquinolines via [5+1] annulation of 2-alkynylanilines and $CFBr_3$ has been developed using N-methylmorpholine (NMM) and photonic energy. Under visible light irradiation, photoinduced charge-transfer of a $CFBr_3$–NMM halogen bond (XB) complex generates •$CFBr_2$ and •Br–NMM radicals, which undergo alkyne addition and halogen atom transfer (XAT) to furnish the atom-transfer radical addition (ATRA) product en route aromatization. After the XAT reaction, ATRA products are created and NMM is regenerated. NMM is used as a catalyst to participate in the reaction cycle again. Mechanistic studies suggest that the unprecedented ATRA of 2-aminoarylalkynes is facilitated by the two-center three-electron (2c–3e) interaction between the •$CFBr_2$ radical and the aniline nitrogen atom. With a broad substrate scope, the new reaction not only represents novel de novo entry to 2-fluorinated quinolines but also yields quinoline building blocks possessing 2,4-dihalides that can be converted to a variety of other quinolines.

Poster Presentation : **ORGN.P-370**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nickel-Catalyzed Reductive 1,4-Alkylarylation of 1,3-Enynes to access tetra-substituted allenes

Jihwan Jeon, Sung You Hong*

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

Radical introduction of alkyl iodide to 1,3-enyne followed by formation of allenyl radical shows remarkable possibility of transition metal-catalyzed allene synthesis. However, reductive difunctionalization of 1,3-enyne has not been studied because of its variety of possible undesired products under reductive coupling condition including homo-coupling, di-alky- or di-arylation of 1,3-enyne, vicinal functionalization of 1,3-enyne. Here in, we describe a nickel-catalyzed reductive 1,4-alkylarylation of 1,3-enyne to access structurally diverse tetrasubstituted allenes with high efficiency and regioselectivity. The mechanistic study showed the involvement of Ni(I)–Ar for the activation of alkyl iodide by in situ generation of Ni(I)–Ar

Poster Presentation : **ORGN.P-371**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Water-Augmented Organosuperbase Catalysis to Access β-Functionalized Alkylsulfonyl Fluorides

Jin Hyun Park, Han yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

Sulfur fluoride exchange (SuFEx) reaction, which was revived by Sharpless et al., is identified as a powerful next-generation click-chemistry that enables absolute connectivity. Among SuFExable hubs, ethenesulfonyl fluoride (ESF) and β-substituted ESFs are regarded as highly useful olefin-based platforms, and their utilities had drawn considerable interest from myriad fields of chemistry. Despite sustained attention, successful functionalization of β-substituted ESFs via Michael-type addition reaction is still elusive, due to their intrinsic properties (e.g., low electrophilicity and uncontrollable selectivity). In this symposium, our recent achievements in water-augmented organosuperbase catalyses will be presented. Under "on-water" reaction conditions, highly challenging approaches toward β-functionalized ethanesulfonyl fluorides were achieved by Michael-type (i.e., Michael and aza-Michael) addition reaction. Upon the catalytic systems, remarkably enhanced hydrophobic interactions in the confined hydrophobic shells, which derived from the hydrophobic hydration effects, reinforced reactivities and selectivities. Furthermore, the origin of the hydrophobic amplifications was supported by experimental, analytical, and computational studies.

Poster Presentation : **ORGN.P-372**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Atroposelective and Desymmetric Allylic Alkylation of 2-Arylresorcinols

Kim Sangji, Yongseok Kwon[1,*]

school of pharmacy, Sungkyunkwan University, Korea
[1]*School of Pharmacy, Sungkyunkwan University, Korea*

Atroposelective synthesis of axially chiral biaryls has attracted attention in recent years, owing to their prevalence in natural products and their applications as chiral catalysts and ligands. One promising strategy for introducing axial chirality is the desymmetrization of configurationally stable achiral biaryls, which offers an alternative and attractive approach.The asymmetric palladium catalyzed allylic alkylation is a powerful method for establishing C−C and C−heteroatom bonds. While numerous studies have focused on controlling stereogenic cneters, only a few catalytic methods have been developed for controlling axial chirality. For example, previous research has explored the catalytic control of the C−N axis in non-biaryl anilides, but the asymmetric control of the C−C axis in biaryls has not been thoroughly investigated. In light of this, we developed an atroposelective allylic alkylation of 2-arylresorcinols via desymmetrization. A chiral Pd-phosphoramidite complex was able to distinguish the two prochiral phenolic hydroxyl groups, and subsequent secondary kinetic resolution led to high enantioselectivity (up to 96% ee). To investigate the detailed mechanism of this reaction, computational studies were conducted which provided insight into the origin of enantioselectivity.

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-373**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ortho-Arylation of Polyhalo-Substituted (Hetero)Aryl Tosylates

Eun-Hye Lim, Yong-Ju Kwon, Won-SuK Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The bi(hetero)aryl moiety is a commonly found scaffold in many therapeutic drugs and natural products. Therefore, various synthetic strategies to prepare bi(hetero)aryl moiety have been introduced. Among them, the site-selective Negishi cross-coupling of (hetero)aryl polyhalides has attracted gradually increasing interest. Notably, directing-group mediated ortho-arylation is one of the most used methods. However, directing-group-mediated ortho-metalation is still challenge, due to the competitive elimination of the directing groups. Thus, it is still essential to develop efficient methods for the selective metalation at a desired site of (hetero)aryl polyhalides. Herein, we report the regioselective ortho arylation of polyhalo-substituted (hetero)aryl tosylates using an integrated continuous flow/batch protocol. Formation of arylzinc species under flow conditions is prepared easily and reproducibly in a short residence time. Finally, the method is applied to the synthesis of perampanel, a glutamate receptor antagonist.

Poster Presentation : **ORGN.P-374**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Sustainable Drug Delivery System by the Polymorphic Transition of Hexagonal Foldectures

Jae-Hoon Eom, Jintaek Gong[1], Jaewook Kim, Hee-Seung Lee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemical Science Education, Sunchon National University, Korea*

Polymorphic phase transitions are very interesting features of organic and inorganic crystals in which part or whole molecules undergo conformational changes by specific activation energies. Controlling the speed and shape of polymorphic transitions is a very challenging from both a scientific and applied point of view. Herein, we report a sustainable drug delivery system by the polymorphic transition of the hexagonal foldectures. Hexagonal prism shaped foldectures change parallelogram plate shapes, which were possible without external stimulation. Transition speed can be controlled to changes in the external environment. The mechanism for dissociation and reassembly was proposed by monitoring the polymorphic transition process in real time with an optical microscope. The PXRD and DSC revealed important information on the intermolecular packing mode and thermal stability of two foldectures. In addition, we confirmed that shape transformation is possible in vivo by mouse experiment.

Poster Presentation : **ORGN.P-375**

Organic Chemistry

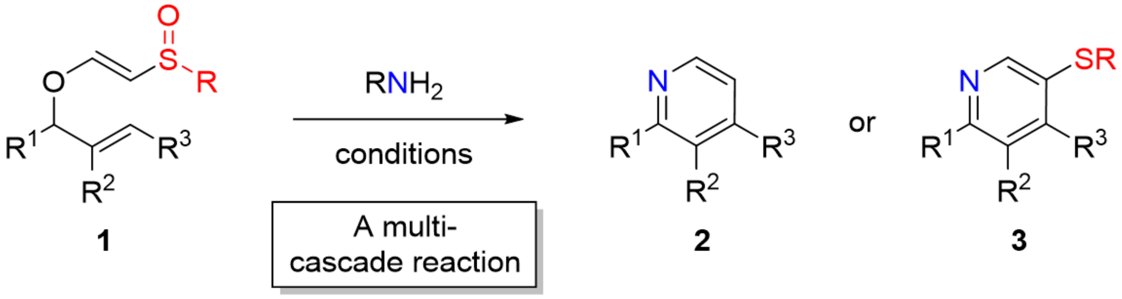
Exhibition Hall 2+3 (1F) THU 11:00~13:00

A New Multi-Cascade Method for the synthesis of Highly Substituted Pyridine

Hyunghwan Seo, Jaehee Kim, Yonghoon Kwon*

Department of Agricultural Biotechnology, Seoul National University, Korea

Pyridines are commonly found in natural products and are often used as ligands or catalysts. Although various methods exist for synthesizing pyridines, the synthesis of highly substituted pyridines has been limited.We recently developed a new multi-cascade method for synthesizing pyridines. We used vinylcarbinoxy vinyl sulfoxide 1 under thermal conditions to synthesize highly substituted pyridine 2 through a series of reactions including Claisen rearrangement, sulfoxide elimination, imine condensation, 6-π electrocyclization, and auto-oxidation. Furthermore, a modification of the reaction conditions brought the additional incorporation of a thioether group at the inactive C-3 position, resulting in compound 3. This introduction was made by highly unprecedented recycling processes of the sulfoxide elimination. We share ongoing efforts and mechanistic details in this talk.



Poster Presentation : **ORGN.P-376**

Organic Chemistry

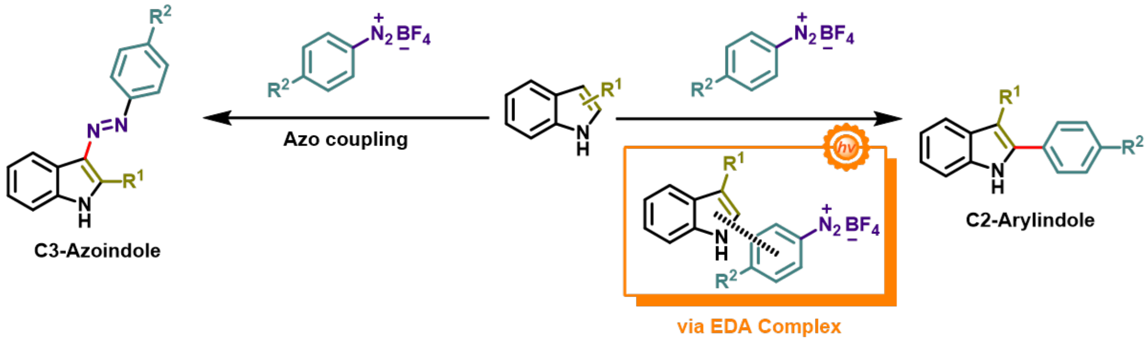
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Chemoselective Arylation and Azo Coupling of Indoles using Aryl Diazonium Salts.

Yuri Kim, Minju Jin, Eun Joo Kang[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Indole scaffolds are widely distributed in nature and they exhibit a broad range of biological activities.Thus, the development of efficient and convenient methods for functionalization of indoles is of great importance. During the past few decades, functionalization of indoles has advanced as an attractive strategy[1], but there have been no pioneering results on different functionalizations of indole from the same material.Aryl diazonium salts are versatile building blocks in organic synthesis. The reaction of aryl diazonium salts can be categorized into two classes, including transformations via aryl radical and transformations with retention of the dinitrogen group.[2]Herein, we designed the C2 arylation and C3 azo coupling of indoles by a selective transformation of aryl diazonium salts without the need for an additional metal, photocatalyst, additives. Under very similar reaction conditions, indoles can be photochemically converted to arylindoles via electron-donor acceptor (EDA) complex or form azoindoles in the absence of a light source. Azoindole and arylindole products are extremely important because of their good anti-tumor activity in vitro[3],[4], and additional subsequent mechanistic studies and substrate expansions are still ongoing.



☐ mild and simple conditions ☐ metal/photocatalyst free ☐ oxidant/base free ☐ direct C(sp^2)-N(sp^2), C(sp^2)-C(sp^2) bond formation

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Poster Presentation : **ORGN.P-377**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Thiazole Derivative of Spiropyran as Metal Sensor

Eun Ju Shin

Department of Chemistry, Sunchon National University, Korea

Spiropyrans are typical photoswitchable compounds, whose molecular structure can be changed after exposure to various external stimuli. They would undergo reversible structural transformation between a colourless ring-closed SP form and a coloured ring-opened merocyanine (MC) form upon light, temperature, pH, chemical species, or mechanical forces, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range. Various metals, especially transition metals and heavy metals, play an important role in biological, environmental, material, and industrial fields. Metal cation driven photochromic transformation of spiropyran has been incredibly widely used for detecting various metals. A variety of spiropyran derivatives has been extensively studied since first discovery in the early 20th century and its photochromism discovered in 1952, due to their versatile application in diverse fields. However, there are few studies on benzothiazole derivatives. In this study, a thiazole derivative of spiropyran was synthesized and characterized. It is interesting to investigate, based on the absorption and fluorescence spectra, how the presence or absence of sulfur in spiropyran affects the metal sensing ability as well as the photochromic properties.

Poster Presentation : **ORGN.P-378**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Rh(III)-Catalyzed C−H Alkylation of 4-Quinolones and Hetero-Aryl Migration: Mechanistic Understanding of Hetero-Aryl Migration

Yelim Kim, Juhyun Kim[1,*]

Department of Chemistry (BK21 FOUR), Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

Transition metal-catalyzed direct C–H bond activation has become an important synthetic strategy in terms of high step- and atom-economy. The direct functionalization of inert C–H bonds is one of the most straightforward approaches to increase molecular complexity in organic synthesis. In this area, directing groups (DGs) not only enhance reactivity, but also solve the problem of regioselectivity in organic molecules containing multiple C–H bonds. Nevertheless, they always bring chemical traces in products, which limits the structural diversity. For the sake of overcoming the disadvantage, some strategies have been devised, including the incorporation of DG into the product via C–H bond activation/DG migration. Various migrating groups, such as oxy, amido, phthaloyl, heteroaryl, carbamoyl, and nitroso groups, have been developed. Among them, hetero-aryl migration usually takes mainly the following three pathways : (i) *via* a C–H activation/Smiles rearrangement cascade by taking advantage of the high nucleophilicity of C–TM bond (ii) *via* base-mediated deprotonation/nucleophilic substitution (iii) *via* acid-promoted hetero-aryl rearrangement. Herein, we report Cp*Rh(III)-catalyzed C–H alkylation of 1-(pyrimidin-2-yl)quinolin-4(1*H*)-one (1) and directing group migration. The C–H alkylation of 4-quinolones 1 proceeded using non-polar solvent, whereas, sequential C–H alkylation/directing group migration proceeded using polar solvent without additional base. For the understanding of the unusual hetero-aryl rearrangement, mechanistic studies are being conducted.

Poster Presentation : **ORGN.P-379**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

[Withdrawal] Divergent synthesis of 2H-pyrrole and 1H-pyrrole via Pd-catalyzed [3+2] cycloaddition

Joungun Park, **Juhyun Kim**[1,*]

Department of Chemistry (BK 21 FOUR), Gyeongsang National University, Korea

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

Poster Presentation : **ORGN.P-380**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhanced Reverse Intersystem Crossing in Halogenated Organic Emitters

Youngnam Lee, Jong-in Hong[*]

Chemistry, Seoul National University, Korea

We synthesized halogen-substituted multiple-resonance (MR) thermally activated delayed fluorescence emitters, namely 2,12-dichloro-*N*,*N*,5,9-tetrakis(4-chlorophenyl)-5,9-dihydro-5,9-diaza-13*b*-boranaphtho[3,2,1-*de*]anthracen-7-amine (Cl-MR) and 2,12-dibromo-*N*,*N*,5,9-tetrakis(4-bromophenyl)-5,9-dihydro-5,9-diaza-13*b*-boranaphtho[3,2,1-*de*]anthracen-7-amine (Br-MR). Cl-MR and Br-MR exhibited a decreased delayed fluorescence lifetime and an enhanced reverse intersystem crossing rate without any changes in ΔE_{ST} and orbital distribution compared with a non-halogenated MR emitter. Cl-MR exhibited a high photoluminescence quantum yield (PLQY) of 85% and external quantum efficiency (EQE) of 17%; however, Br-MR did not exhibit any enhancement in the PLQY and EQE. The different performances of Cl-MR and Br-MR were rationalized by analysing the rate constants of the excited states and bond dissociation energies of the carbon–halogen bonds.

Poster Presentation : **ORGN.P-381**

Organic Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

A blue emitter with thermally activated delayed fluorescence utilizing a rigid electron acceptor and multiple electron donors

Youngnam Lee, Jiyun Kim, Jong-in Hong*

Chemistry, Seoul National University, Korea

Thermally activated delayed fluorescence (TADF) has emerged as a promising approach to enhance the internal quantum efficiency (IQE) and external quantum efficiency (EQE) of organic light-emitting diodes (OLEDs). To achieve this, a rigid molecular structure is required to improve the IQE and narrow the emission spectrum. Recently, a rigid electron acceptor, 5,9-dioxa-13*b*-boranaphtho[3,2,1-*de*]anthracene (OBO), was used to synthesize TADF emitters that demonstrated high EQEs and narrow full width at half maximum (FWHM). Our study utilized multiple 3,6-di-*tert*-butyl-9*H*-carbazoles as electron donors and OBO as the electron acceptor to synthesize 9,9',9''-(5,9-dioxa-13*b*-boranaphtho[3,2,1-*de*]anthracene-3,7,11-triyl)tris(3,6-di-*tert*-butyl-9*H*-carbazole) (OBO3tCz). This new molecule exhibited a maximum emission wavelength (λ_{max}) of 426 nm, FWHM of 41 nm, and the energy difference between singlet and triplet states (ΔE_{ST}) of 0.16 eV, which is sufficient for TADF emission. Additionally, a 10% doped film in bis[2-(diphenylphosphino)phenyl] ether oxide (DPEPO) showed a high photoluminescence quantum yield (PLQY) of 90% and clear TADF emission. Consequently, an OLED device incorporating OBO3tCz achieved a high EQE of 23% and blue color emission at 460 nm.

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Poster Presentation : **ORGN.P-382**
Organic Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of symmetrical bisindolizine framework via metal-catalyzed dehydrogenativeapproach: A new entry for AIEgens

Eunha Kim

Department of Molecular Science and Technology, Ajou University, Korea

Indolizine is one of the intrinsically fine-tunable fluorescent skeletons display versatile bioimaging and materialapplications. On the other hand, most conventional fluorophores exhibit aggregation caused quenching but fewfluorophores showed increased emission in their aggregated or solid-state forms known as aggregation inducedemission (AIE). Very recently, indolizine based color tunable AIEgens are discovered and explored for thevisualization of mitochondria and endoplasmic reticulum. In line with this, our ongoing research is based on theinvestigation of symmetrical indolizine and its photophysical properties. Therefore, we envisioned to develop a series of new symmetrical bisindolizine framework as an AIEgen using metal-catalyst. Detailed synthesis and photophysical properties of the newly prepared molecules will be discussed in the poster presentation.

Poster Presentation : **MEDI.P-383**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ethanol extract of Polyscias fruticosa attenuated glutamate induced neuronal cell death in vitro and in vivo study

Baskar Selvaraj, Ae Nim Pae[1], Jae Wook Lee[2,*]

natural product research center, Korea Institute of Science and Technology, Korea
[1]Korea Institute of Science and Technology, Korea
[2]Natural Product Research Center, Korea Institute of Science and Technology, Korea

Polyscias fruticosa, known as traditional medicine, has been frequently used for the treatment of ischemia and inflammation. However, little research has investigated the neuroprotective effects of Polyscias fruticosa. The current study aimed to identify the neuroprotective effect of ethanol extract Polyscias fruticosa (EEPF) and elucidate the underlying mechanism of neuroprotective of EEPF in vitro and in vivo. The effects of EEPF on the neuroprotection was determined by measuring cell viability. Protein expression of AKT, BDNF, CREB, Bax, Bcl-2 and apoptosis inducing factor (AIF) were determined by western blot analysis. The ratio of apoptotic and death cells were evaluated by flow cytometry. Cellular Ca2+ level and reactive oxygen species (ROS) level were measured using fluor-3 and 2',7'-dichlorodihydrofluorescein diacetate, respectively. In vivo efficacy of EEPF was evaluated using the monglian gerbil by inducing brain ischemia. EEPF treatment shows neuroprotective effect against glutamate induced cell death. p-AKT, p-CREB, BDNF and Bcl-2 were decreased by glutamate treatment and gradually increased by EEPF cotreatment. Bax and AIF were increased by glutamate and gradually decreased by EEPF cotreatment. Ratio of apoptosis and death cells were decreased by the treatment of EEPF. Cellular Ca2+ and ROS level were decreased by EEPF treatment. In vivo efficacy data indicated that EEPF treatment diminished the number of degenerative neurons. EEPF exhibited neuroprotective properties that suppress glutamate-mediated neurotoxicity. The underlying mechanism of EEPF is increasing level of p-AKT, p-CREB, BDNF, and Bcl-2, which are related with cell survival. EEPF decreases the level of Bax and AIF translocation.

Poster Presentation : **MEDI.P-384**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Identification of TRD-93 as a novel DRAK2 inhibitor

Seungmin Kye, Kwangho Lee[1,*]

University of Science & Technology, Korea
[1]*Korea Research Institute of Chemical 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 enriched in B and T cells for possible immunological responses: DRAK2-deficient knock-out mice develop resistance to autoimmune diseases such as EAE (experimental autoimmune encephalomyelitis) and type I diabetes. In addition, 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 autoimmune diseases and cancers. 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 singleton 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 poster presentation, we report TRD-93 is potent and selective DRAK2 inhibitor (IC_{50} = 0.16 μM) and its molecular binding mode.

Poster Presentation : **MEDI.P-385**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of Potent Inhibitors Targeting Phosphopantetheinyl Transferase

Sang keun Lee[*], **Kyumyung Lee**[*]

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

Tuberculosis (TB) is a potentially serious infectious disease usually caused by *Mycobacterium tuberculosis* (Mtb) bacteria that mainly affects the lungs, but can affect any part of the body including the tummy, glands, and nervous system. About one-quarter of the world's population has a TB infection, which means people have been infected by TB bacteria but are not (yet) ill with the disease and cannot transmit it. It is called latent TB, which could develop into an active TB at a later date, particularly if immune system becomes weakened. Effective TB treatment is difficult, due to the unusual structure and chemical composition of the mycobacterial cell wall, which hinders the entry of drugs and makes many antibiotics ineffective. Biosyntheses of the cell wall components and small molecule virulence factors require large multidomain synthases containing carrier protein (CP) domains. CPs tether the elongating product through a thioester linkage to a posttranslationally attached 4´-phosphopantetheinyl group. Post-translational modifications are carried out by Mg^{2+}-dependent 4´-phosphopantetheinyl transferases (PptT). PptT attaches the 4´-phosphopantetheine arm of coenzyme A (CoA) to a conserved serine residue of the CP. Therefore, inhibiting PptT is a novel target for treatment of TB. We discovered a hit via high throughput screening (HTS) and synthesized several compounds derived from it. Among them, five compounds showed good inhibitory activity in PptT more than the reference compound reported in Science. We are currently producing further modification of them that will be examined in the near future.

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Poster Presentation : **MEDI.P-386**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Molecular Docking Study new quinolone-based diarylamides as potent B-RAF(V600E)/C-RAF kinase inhibitors

Jung Woo Park

Korea Institute of Science and Technology Information, Korea

Molecular docking, which models the interaction between the target protein and the inhibitor at the atomic level and analyzes the binding mode, helps a lot in understanding the inhibitor's structure-activity relationship. In particular, thanks to the enhancement of computing power and the development of analytical equipment technologies such as X-ray crystallography and NMR, more accurate structural predictions and faster calculations are possible, making it widely used in the development of new drugs.A docking study was conducted to elucidate the activity of quinolone-based derivatives from a structural point of view. BRAFV600E (PDB code: 1UWJ) and CRAF homology models were utilized. The molecular docking studies were performed by sequentially inserting candidate substances into the sorafenib binding site of RAF kinase. In this study, as well as analyzing important common ligand-protein binding, structural differences of candidates affecting the inhibitory effect of RAF kinase were revealed through the binding mode.

Poster Presentation : **MEDI.P-387**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Cancer-specific cytotoxicity of pyridinium-based ionic liquids by regulating hypoxia-inducible factor-1α-centric cancer metabolism

Beomchan Seo, Taejin Ha[1], Jong dae Lee[*]

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

Owing to their unique properties and biological activities, ionic liquids (ILs) have attracted research interest in pharmaceutics and medicine. Hypoxia-inducible factor (HIF)− 1α is an attractive cancer drug target involved in cancer malignancy in the hypoxic tumor microenvironment. Herein, we report the inhibitory activity of ILs on the HIF-1α pathway and their mechanism of action. Substitution of a dimethylamino group on pyridinium reduced hypoxia-induced HIF-1α activation. It selectively inhibited the viability of the human colon cancer cell line HCT116, compared to that of the normal fibroblast cell line WI-38. These activities were enhanced by increasing the alkyl chain length in the pyridinium. Under hypoxic conditions, dimethylaminopyridinium reduced the accumulation of HIF-1α and its target genes without affecting the HIF1A mRNA level in cancer cells. It suppressed the oxygen consumption rate and ATP production by directly inhibiting electron transfer chain complex I, which led to enhanced intracellular oxygen content and oxygen-dependent degradation of HIF-1α under hypoxia. These results indicate that dimethylaminopyridinium suppresses the mitochondria and HIF-1α□dependent glucose metabolic pathway in hypoxic cancer cells. This study provides insights into the anticancer activity of pyridinium-based ILs through the regulation of cancer metabolism, making them promising candi□dates for cancer treatment

Poster Presentation : **MEDI.P-388**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of indole analogs as PIM kinase inhibitors

Jieun Kim, Mingyu Jeon, Dagyu Kang, Victor Sukbong Hong*, Jinho Lee*

Department of Chemistry, Keimyung University, Korea

PIM (Proviral Integration Site for Moloney Murine Leukemia Virus) kinase is a member of the serine/threonine kinase family and comprises three isoforms: PIM-1, PIM-2, and PIM-3. These kinases play important roles in regulating cellular processes, including cell proliferation, transcription, survival, cell cycle regulation, metastasis, and apoptosis. Abnormal expression of PIM kinases is associated with various types of cancer, including hematological and solid tumors. As a result, PIM kinases are considered a potential target for developing anticancer drugs.In this study, indole derivatives were synthesized and evaluated for their potential as PIM kinase inhibitors. The structure-activity relationship was analyzed by introducing diverse substituents at the 3- and 5-positions of the indole ring. The inhibitory activity of the compounds was found to be influenced by the hydrophilic and lipophilic properties of each substituent. The most potent inhibitor showed IC_{50} values of 0.6 nM and 1.0 nM for PIM-1 and PIM-3, respectively.

Poster Presentation : **MEDI.P-389**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthetic Cinnamaldehyde Derivatives Targeting TRPA1 in Schwann Cells Regulates Wallerian degeneration

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Anatomy and Neurobiology, Kyung Hee University, Korea

Peripheral nerve degeneration (PND) is a preparative process for peripheral nerve regeneration and is regulated by Schwann cells, a unique glial cell in the peripheral nervous system. Dysregulated PND induces irreversible peripheral neurodegenerative diseases (e.g., diabetic peripheral neuropathy). To develop novel synthetic drugs for these diseases, we synthesized a set of new cinnamaldehyde (CAH) derivatives and evaluated their activities *in vitro*, *ex vivo*, and *in vivo*. The 12 CAH derivatives had phenyl or naphthyl groups with different substitution patterns on either side of the α,β-unsaturated ketone. Among them, 3f, which had a naphthaldehyde group, was the most potent at inhibiting PND *in vitro*, *ex vivo*, and *in vivo*. To assess their interactions with transient receptor potential cation channel subfamily A member 1 (TRPA1) as a target of CAH, molecular docking studies were performed. Hydrophobic interactions had the highest binding affinity. To evaluate the underlying pharmacological mechanism, we performed bioinformatics analysis of the effect of 3f on PND based on coding genes and miRNAs regulated by CAH, suggesting that 3f affects oxidative stress in Schwann cells. The results show 3f to be a potential lead compound for the development of novel synthetic drugs for the treatment of peripheral neurodegenerative diseases.

Poster Presentation : **MEDI.P-390**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Design, Synthesis and Biological Evaluation of Novel Microtubule-Targeting Agent Based on Bioactive Conformation

Jaebeom Park, Minji Kang[1], Yeju Oh[1], Hongjun Jeon[1,*]

Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology (KRICT), College of Pharmacy, Chungbuk National University, Korea

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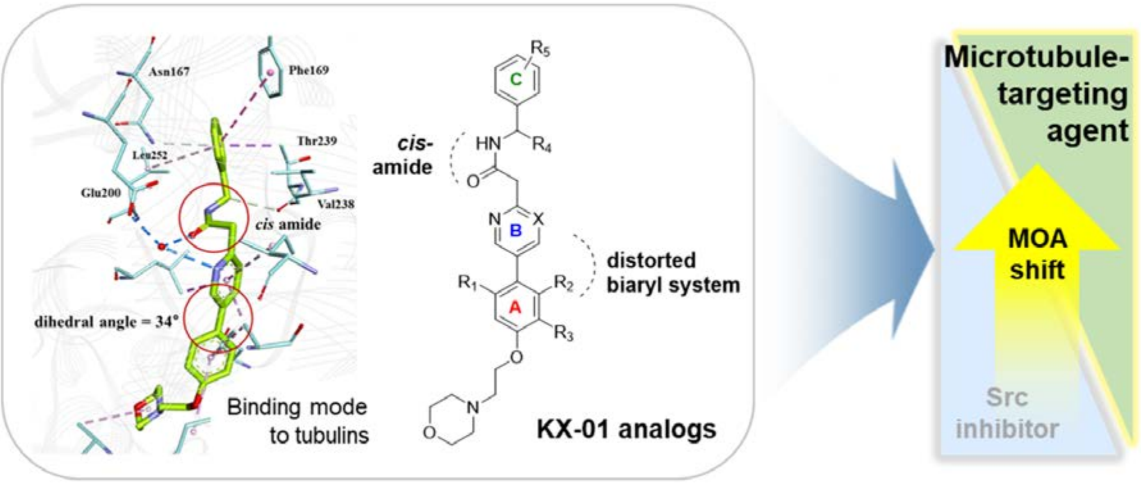
Microtubule-targeting agents (MTAs) are a crucial component in the fight against cancer. These chemotherapy agents work by promoting apoptosis through stabilizing or destabilizing microtubules in order to arrest the cell cycle in the G2/M phase. Tirbanibulin (KX-01) was approved by the FDA in 2020 as a first-in-class treatment for pre-cancerous actinic keratosis on the face or scalp, but it has not yet been approved for use as an anticancer drug due to limited efficacy in a phase 2 clinical trial for metastatic castration-resistant prostate cancer patients (NCT01074138). Tirbanibulin has two unique mechanisms of action: Src inhibition and tubulin destabilization. We have focused on microtubule inhibition to develop it as a payload for antibody-drug conjugate payload. Two main strategies were used to increase its potency: 1) "locking" the molecule in its bioactive conformation, and 2) mimicking the dihedral angle of the biaryl system (A and B ring) of KX-01 as seen in its co-crystal structure (PDB code: 6KNZ). Numerous analogs have been synthesized and evaluated based on these strategies.


Asn167
Phe169
Thr239
Leu252
Glu200
Val238
cis amide
dihedral angle = 34°
Binding mode
to tubulins
cis-
amide
R_5
C
HN
R_4
O
N
B
X
R_1
R_2
A
R_3
O
N
O
distorted
biaryl system
KX-01 analogs
Microtubule-
targeting
agent
MOA
shift
Src
inhibitor

Poster Presentation : **MEDI.P-391**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of multifunctional silica nanoparticles as cancer-specific theranostics.

Hyeungjun Kim, InCheol Heo[1,*], Won Cheol Yoo[2,*], Sun-Joon Min[3,*]

Applied chemistry, Hanyang University, Korea
[1]*Department of Applied chemistry, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*
[3]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

A number of nanomaterials are being used as drug-delivery vehicles over the last few decades due to their potential for facile structural modification, biocompatibility and target specificity. In this study, we present development of multifunctional silica nanoparticles (SNPs) as diagnostic and therapeutic materials that will be able to simultaneously visualize and treat various diseases, such as cancer. We designed and synthesized multimodal SNPs consisting of three components, namely, folic acid, camptothecin and Cy 5.5 fluorescence dye. Initially, the Cy 5.5 dye was incorporated into SNPs for fluorescent imaging by modified Stöber method. According to our procedure reported in the previous publication, a bismethallyl silane linker was prepared, having folic acid (FA) as a target-specific ligand for FA receptors on cancer cell surfaces, and camptothecin (CPT) as a chemotherapeutic reagent. CPT was conjugated with the linker to form thioether or disulfide bond, which enables our SNPs to perform intracellular controlled drug release. The silane linker was successfully introduced onto the surface of monodispersed SNPs via Sc(OTf)3-catalyzed siloxane formation. Finally, the in vitro studies showed that our multifunctional SNPs exhibited high chemotherapeutic effects on cancel cells due to their high cellular-uptake properties through receptor-mediated endocytosis.

Poster Presentation : **MEDI.P-392**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Benzamide derivative, AI-assisted de novo design approach to design a selective inhibitor for FLT-3(D835Y) in acute myeloid leukemia

Eun gyeong Shin

Therapeutics & Biotechnology , Korea Research Institute of Chemical Technology, Korea

Acute myeloid leukemia (AML) is a hematological malignancy that causes abnormal proliferation and differentiation of bone marrow cells. FLT3 is a member of the III receptor tyrosine kinase family and plays an important role in regulating the survival, proliferation and differentiation of hematopoietic stem cells. Therefore, targeting FMS-like tyrosine kinase 3 (FLT-3) and its mutations to treat acute myeloid leukemia (AML) is an effective therapeutic strategy. FLT3 mutations consist of an internal tandem duplication (ITD) mutation and a tyrosine kinase domain (TKD) mutation, of which the FLT-3 point mutation is commonly found in AML and occurs at inactivating loop residue D835, stabilizing the inactive conformation. In this study, we discovered novel and highly selective compounds with desired drug-like properties targeting the FLT-3(D835Y) mutation using AI-assisted hit optimization. Among these compounds, PCW-A1001 proved highly selective for the FLT-3(D835Y) mutant, with an IC50 of 2.54 μM versus 764 nM for FLT-3 WT.

Poster Presentation : **MEDI.P-393**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Inhibition of cancer growth and progression via targeting of mitochondrial respiration and reduction of HIF-1α accumulation using LW1564

Min kyoung Kim, Kyeong Lee*

College of Pharmacy, Dongguk University, Korea

The hypoxic tumour microenvironment promotes the malignant phenotype of cancer cells by inducing the expression of genes involved in metabolism, angiogenesis, metastasis and resistance to cell death. Targeting cancer metabolism has emerged as an important cancer therapeutic strategy. Here we describe the synthesis and biological evaluation of a novel class of hypoxia-inducible factor (HIF)-1α inhibitors, disubstituted adamantyl derivatives.LW1564 promoted the phosphorylation of acetyl-CoA carboxylase, which inhibited lipid synthesis. In addition, LW1564 significantly inhibited tumour growth in a HepG2 mouse xenograft model. Taken together, the results indicate that LW1564 inhibits the growth of cancer cells by targeting mitochondrial ETC complex I and impairing cancer cell metabolism. We therefore suggest that LW1564 may be a potent therapeutic agent for a subset of cancers that rely on oxidative phosphorylation for ATP generation.

Poster Presentation : **MEDI.P-394**
Medicinal Chemistry
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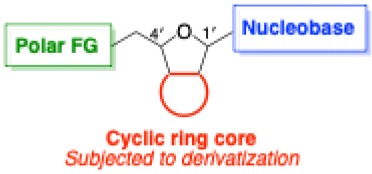
Progress in discovery of a novel antibiotic featuring the nucleoside structure to combat against non-tuberculosis mycobacteria (NTM)

Yujin Jung, Hak Joong Kim[*]

Department of Chemistry, Korea University, Korea

The infection caused by non-tuberculosis mycobacteria (NTM) is hard to treat mainly because of the development of resistance against antibiotics and the lack of reliable treatment regime. Hence, a new antibiotic targeting NTM should be able to effectively address such problems associated with the antibiotic resistance of NTM. In our preliminary library screening, a unique compound featuring the nucleoside structure was identified as a potent hit against *Mycobacterium abscessus*, one of NTM, leading us to pursue the structure-activity relationship study based thereon. Before embarking on extensive analogue generation, it was attempted to establish the effect of the stereochemistry at 1′ and 4′-positions of the hit nucleoside molecule on the biological activity. Accordingly, four stereoisomers of the base structure were synthesized, and then the activity of each pure stereoisomers was tested against *M. abscessus* and *M. avium*, demonstrating that the (1′*R*,4′*R*)-*trans*-isomer could exhibit higher activity than the other stereoisomers. Furthermore, an SAR study was conducted particularly on variation of the fused cyclic ring core, and this presentation will detail our current observations on the antibiotic activity of these analogues.



Poster Presentation : **MEDI.P-395**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Novel NUAK1 Inhibitor for Treatment of Pancreatic Cancer

Kewon Kim, Sungwoo Hong[*]

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

The novel (nua) kinase family 1 (NUAK1) is an AMPK-related kinase and its expression is associated with tumor malignancy and poor prognosis in various types of cancer. This suggests NUAK1 can be a promising target for cancer therapy. We synthesized KI-301670, a novel NUAK1 inhibitor, and observed its anticancer ability and mechanism of action in pancreatic cancer development. It effectively inhibited pancreatic cancer growth and proliferation, and induced cell cycle arrest, markedly G0/G1 arrest, by increasing the expression of p27 and decreasing expression of p-Rb and E2F1. Furthermore, the apoptotic effect of KI-301670 was observed by an increase in cleaved PARP, TUNEL-positive cells, and annexin V cell population, as well as the release of cytochrome c via the loss of mitochondrial membrane potential. KI-301670 inhibited the migration and invasion of pancreatic cancer cells which are important of cancer metastasis. Mechanistically, KI-301670 effectively inhibited the PI3K/AKT pathway in pancreatic cancer cells. Notably, it significantly attenuated tumor growth in a mouse xenograft tumor model. These results demonstrate that a novel NUAK1 inhibitor, KI-301670, exerts promising anti-tumor effects by directly suppressing cancer cell growth by affecting the PI3K/ AKT pathway, suggesting that it could be a novel therapeutic candidate for pancreatic cancer treatment.

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Poster Presentation : **MEDI.P-396**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of selective histone deacetylase inhibitors and its biological effects in microglia

Shinhyeong Kim, Jonghoon Kim*

Department of Chemistry, Soongsil University, Korea

Histone deacetylases (HDACs) are key epigenetic regulators, and the 18 different HDAC isoforms are classified into four subtypes. Despite the various roles of each HDAC isoform, the lack of selective HDAC inhibitors has limited the elucidation of their individual roles. We developed HDAC inhibitors with (aryloxopropenyl)pyrrolyl hydroxamates scaffold and demonstrated that HDAC inhibitor 1 initiated autophagy and suppressed lipopolysaccharide-induced neurotoxicity in microglia via regulation of the deacetylase function of HDAC11. Furthermore, we generated another compound libraries structurally related to HDAC inhibitor 1 and evaluated its inhibitory activity against HDACs and therapeutic potential in human microglia.

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Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of microglial activation inhibitors for neuroinflammation-associated diseases treatment

Jun Hyeok Son, Sanghee Lee[1,*]

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Neuroinflammation is an initial defense mechanism that protects the central nervous system by suppressing and eliminating various pathogens. However, chronic neuroinflammation can induce neuronal death, and the accumulation of neuronal damage accelerates neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, and amyotrophic lateral sclerosis. Therefore, inhibition of inflammatory response in chronic neuroinflammation is essential to prevent the development of neurodegenerative disorders. Various brain cells, such as neurons, microglia, and infiltrating leukocytes, are associated with neuroinflammation. Specially, microglia are considered the key regulator of neuroinflammation since they are in the brain and play a role in neuroprotection by producing pro-inflammatory cytokines in response to various pathogens. Moreover, chronic microglial activation can lead to neurotoxicity, which shows the important role of microglia in neuroinflammation. In this study, we focused on finding a new inhibitor of microglial activation to suppress neuroinflammation. Our specific core compounds showed inhibition of microglial activation, which led to the alleviation of neuronal death.

Poster Presentation : **MEDI.P-398**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a Novel HDAC inhibitor Exhibiting Therapeutic Potential to Prevent Depression via HDAC11 Inhibition in Microglia

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Histone deacetylases (HDACs) are key epigenetic regulators and classified into four subtypes. Despite the various roles of each HDAC isoform, the lack of selective HDAC inhibitors has limited the elucidation of their individual roles in biological systems. HDAC11, the sole class-IV HDAC, is highly expressed in brain, however, the role of HDAC11 in microglia is not fully understood. Based on the modification of MC1568, we develop a novel HDAC inhibitor, 5. Interestingly, 5 suppresses lipopolysaccharide-induced microglial activation by the initiation of autophagy and subsequent inhibition of nitric oxide production. Furthermore, we demonstrated that 5 significantly alleviates depression-like behavior by suppression of microglial activation in mouse brain. Our discovery of HDAC11 inhibitor reveals the role of HDAC11 in autophagy and reactive nitrogen species balance in microglia for the first time, which makes HDAC11 a new therapeutic target for depressive disorder.

Poster Presentation : **MEDI.P-399**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Paeonol-tryptamine hybrid compounds for selective butyrylcholinesterase inhibitors

Minji Kim, Sung Ha Hwang, Jeong Ho Park*

Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea

The paeonol structure exhibits pharmacological activities such as anti-ChE activity, anti-inflammatory, reduced cerebral infarction, and anti-mutagenesis. Triazole derivatives exhibit pharmacological activities such as antibacterial, anti-parasitic, antidiabetic, painkillers and anti-inflammatory. Based on the cholinergic theory for the treatment of Alzheimer's disease (AD), we explored new cholinergic inhibitors. This study used various benzyl intermediates in place of the methyl group of methoxy at position 4 of paeonol. Paeonol-tryptamine hybrid compounds were synthesized through click reaction using paeonol derivatives and tryptamine. They showed an inhibitory effect on butyrylcholinesterase (BuChE) rather than acetylcholinesterase (AChE). Compound 33 (IC$_{50}$=0.21 ± 0.12 μM for BuChE) showed better inhibitory activity than the positive control galantamine (IC$_{50}$=12.74 ± 0.36 μM for BuChE).

Poster Presentation : **MEDI.P-400**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Exploring the pKa values and physicochemical properties of phlorotannin compounds in brown algae

Mingyeong Kim, Bong Ho Lee*, Byong Wook Choi, Hyeon Cheol Shin[1], Hyejeong Hwang[1]

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[1]*Center for Molecular Intelligence, The State University of New York, Korea (SUNY Korea), Korea*

Brown algae have various secondary metabolites, including several polyphenolic compounds known as phlorotannins. Among them, dieckol (DE) is the most abundant and widely known compound, with 11 -OH groups and diverse physiological activities such as antioxidant, anti-inflammatory, and enzyme inhibitory activities. Despite its promising physiological activities and safety, the basic physicochemical properties of this compound are not well-known. Therefore, we investigated the acidity (pKa) and stability of several types of phlorotannins at different pH and the presence of oxygen. Our UV-visible spectrum showed that dieckol is relatively stable under acidic conditions, but undergoes structural changes under alkaline conditions, causing a rapid change in the spectrum. The pKa of dieckol, determined by the absorbance changes, was found to be 8.08 ± 0.5, which is lower than the known pKa of polyphenols, which is approximately 10. According to our results, the pH of the buffer solution used in most physiological activity measurement methods using enzymes is between 6 and 9, indicating that dieckol may have already undergone protonation or deprotonation or may exist in a different form during the analysis process.These results suggest that dieckol may exhibit different activities than those known when absorbed into the body as an effective ingredient in functional foods or medicines. Our study aims to verify the structural stability of phlorotannins, including dieckol, according to their acidity and to determine the changes in structure and activity.

Poster Presentation : **MEDI.P-401**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

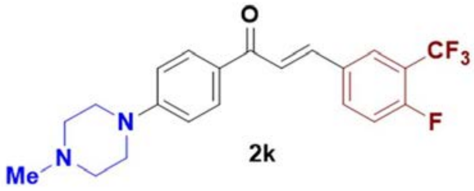
Identification of new Fluoriated chalcones with N-methyl-piperazine as dual MAO-B/AChE inhibitors

Ashraf El-Damasy, Gyo chang Keum[1,*]

Department of Medicinal Chemistry, Faculty of Pharmacy, Egypt
[1]*Chemoinformatics Research Center, Korea Institute of Science and Technology, Korea*

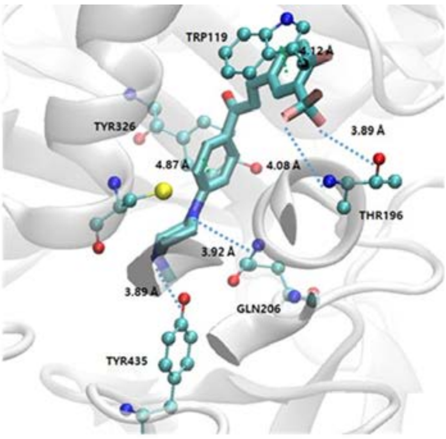
Monoamine oxidase-B (MAO-B), acetylcholinesterase (AChE), and butyrylcholinesterase (BChE) have been considered target enzymes of depression and neurodegenerative diseases including Alzheimer’s disease (AD). In this study, seventeen N-methyl-piperazine chalcones were synthesized and their inhibitory activities were evaluated against the target enzymes. Compound 2k (3-trifluoromethyl-4-fluorinated derivative) showed the highest selective inhibition against MAO-B with an IC50 of 0.71 μM and selectivity index (SI) of 56.34, followed by 2n (2-fluoro-5-bromophenyl derivative) (IC50 = 1.11 μM, SI = 16.04). Compounds 2k and 2n were reversible competitive MAO-B inhibitors with Ki values of 0.21 and 0.28 μM, respectively. Moreover, 2k and 2n effectively inhibited AChE with IC50 of 8.10 and 4.32 μM, which underscore their multi-target inhibitory mode. Cell-based assay of compounds 2k and 2n against Vero normal cells pointed out their low cytotoxicity. In docking simulation, 2k showed the lowest energy for MAO-B (-11.6 kcal/mol) with four hydrogen bonds and two π-π interactions. Furthermore, in silico studies were conducted, and disclosed that 2k and 2n are expected to possess favorable pharmacokinetic properties, such as the ability to penetrate the blood brain barrier (BBB). In view of these findings, compounds 2k and 2n could serve as promising potential candidates for the treatment of neurodegenerative diseases.

Dual MAO-B/AChE inhibitors

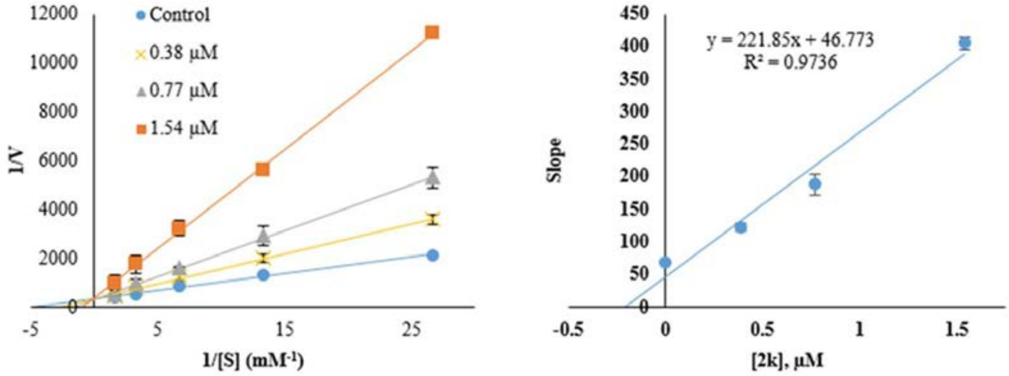


2k

MAO-B, IC_{50} = 0.71 μM, *Ki* = 0.21 μM
AChE, IC_{50} = 8.10 μM
BChE, IC_{50} = 21.1 μM



Docking of 2K with MAO-B



Reversible competitive MAO-B inhibitory mode

Poster Presentation : **MEDI.P-402**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

In silico design and synthesis of NLRP3 inflammasome modulators for treatment of inflammatory diseases

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The NLRP3 (NOD-, LRR- and pyrin domain-containing protein3) inflammasome is a multimeric protein complex that initiates an inflammatory form of cell death and triggers the release of proinflammatory cytokines such as IL-1β and IL-18. Abnormal activation of NLRP3 has been associated with several inflammatory diseases, including cryopyrin syndrome, Alzheimer's, diabetes, and atherosclerosis. Over the past decades, the inflammasome has proliferated as an important innate immune component orchestrating host immune homeostasis. In this study, we show that a peptide fragment 72FYAQFVQALS81, derived from secretion of Mycobacterium tuberculosis (MTB), interacts with the domain of CD86-NLRP3 and inhibits the release of both proinflammatory cytokines IL-1β and IL-18. Based on the structure of this peptide motif, we designed N-heterocycle derivatives as peptide-mimetic small molecules through in silico pharmacophore generation. We conducted a docking study of the designed molecules to the X-crystal structure of NLRP3 protein binding to MCC950, a potent NLRP3 inhibitor. The synthesis and in-vitro evaluation of the compounds with high interaction values in the docking study showed that our compounds not only modulate the NLRP3 inflammasome function, but also reduce reactive inflammatory cytokine production. In this presentation, we will provide a discovery process for peptide-derived small molecules targeting NLRP3 inflammasome for the treatment of inflammatory diseases.

Poster Presentation : **MEDI.P-403**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of a thiol-reactive fluorescence probe selectively targeting gingipains of Porphyromonas gingivalis

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[1]*Department of Bio-Medical Science and Technology, University of Science & Technology, KIST School, Korea*
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Porphyromonas gingivalis is a major pathogen of severe adult periodontitis and was detected in more than 70% of periodontal disease patients. It is a gram-negative oral anaerobe that produces large amounts of Arg- and Lys-specific cysteine proteinases, gingipains, that are responsible for at least 85% of total proteolytic activity exerted by various strains of P. gingivalis. In this work, we developed a thiol-reactive fluorescence probe DTC0630 with more than 6-fold fluorescence activation upon incubation with P. gingivalis. Further in vitro analysis demonstrated the selectivity of the fluorescence 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.

Poster Presentation : **MEDI.P-404**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of lead compounds for the treatment of progressive Supranuclear Palsy by controlling 4R Tauopathy

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Biotechnology, Korea University, Korea

[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

Progressive supranuclear palsy (PSP) is a late-onset degenerative disease that leads to symptoms including loss of balance, slowing of movement, difficulty moving the eyes, and cognitive impairment. However, there is still no treatment for PSP. The cause of the condition involves the accumulation of tau protein within the brain, and brain diseases with abnormal tau deposits are called tauopathies. Tau is a microtubule-associated protein that stabilizes neuronal microtubules. Human tau protein has 6 isoforms, and PSP has a high ratio of 4R tau, which has 4 repetitive microtubule-binding domains. Therefore, we pursued the discovery of novel tau-targeting therapeutic drug candidates for the treatment of PSP, especially 4R tau aggregation inhibitors. To find 4R tau-specific lead compounds, we performed high-throughput screening based on the tau Bi-FC assay with in-house libraries and structural optimization for improvement of in vitro activity and selectivity for 4R tau of hits compounds. Two compounds (DTC 2094 and DTC 2162) showed excellent activity and selectivity for 4R tau over 3R tau. Subsequently, we did in vivo studies in the TauP301L – BiFC mouse model, and these compounds improved motor function in the balance beam test and cognitive impairment in the Barnes Maze test than in the vehicle. We will continue to work further to optimize potency as well as physicochemical properties and toxicity to develop clinical candidates.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **MEDI.P-405**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and anti-inflammatory activity of lithocholic acid derivatives having double bonds in the steroid skeleton

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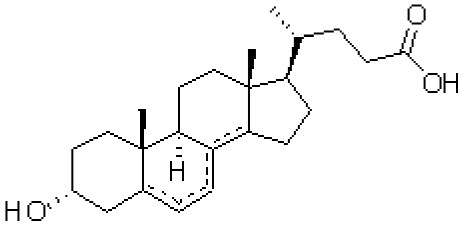
[1]*Department of Chemistry, Kyung Hee University, Korea*

Bile acids are cholesterol-derived natural surfactants produced by the liver and secreted into the duodenum. There are known to function as a major regulator of gut microbiome in addition to their functions as digestive juice that help the absorption of lipids in the intestine. Therefore, bile acids are strong candidates for the treatment of inflammatory bowel disease (IBD) in that they are modulators for the normalization of gut microbiom. As one of the secondary bile acids, lithocholic acid (LCA) formed from chenodeoxycholic acid (CDCA) has been identified as a secondary endogenous agonist of Vitamin D receptor.In this report, the efficient synthesis method of LCA derivatives with a double bond introduced into the steroid backbone is described. In particular, an effective elimination reaction condition for introducing a double bond by removing a C7-hydroxyl group from CDCA will be reported. These derivatives were evaluated for anti-inflammatory activity and compared to LCA and CDCA.



Lithocholic acid derivatives

Poster Presentation : **MEDI.P-406**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of novel small molecule chelator for radiometal-labeled radiopharmaceuticals

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pharmacy, Gyeongsang National University, Korea

1,4,7-Triazacyclononane-1,4,7-triacetic acid and 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid are representative chelators commonly used for labeling of radiometals. However, these chelators may degrade the labeled drug's pharmacological or biological properties due to their structure's polarity. So it is necessary to develop a new chelator that has little effect on the polarity of the target compound. In this study, a pyrrole-based skeletal structure that can easily bind to carboxylic acid was developed, and the potential was evaluated through the chelation of radioactive metals 64Cu and 68Ga as a new chelator. A new chelator with thioryl amide was synthesized from benzoic acid through pivaloyl chloride and triethylamine. Structural analysis was performed by nuclear magnetic resonance (NMR) and liquid chromatography–mass spectrometry (LC–MS). The radiochemical yield and radiochemical purity of the 64Cu or 68Ga chelation complex were confirmed by radio thin layer chromatography (radioTLC).The new chelator was synthesized in 30% yield from benzoic acid. The radiometal 64Cu or 68Ga was chelated with a radiochemical yield of 96% at room temperature in 30 minutes at pH 11, and the radiochemical purity was over 95%. The newly developed chelator successfully chelate radiometals 64Cu and 68Ga using a pyrrole-based skeletal structure. Since this chelator can be labeled under conditions where biological stability is preserved, it is thought that it can be applied from small molecules to antibodies. Thus it has the potential to be a new chelator that can be easily applied to various probes with a carboxylic acid.

Poster Presentation : **MEDI.P-407**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of Thieno[2,3-d]pyrimidine-based Dual Inhibitor for Histone Deacetylase and FLT3-ITD Mutation as Anti-Leukemic Agents

Hao yu Ku, Gyoonhee Han[1,*]

Yonsei University, Taiwan

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

Acute myeloid leukemia (AML) is a hematological disorder characterized by abnormal differentiation and proliferation of clonal hematopoietic stem cells in the bone marrow and peripheral blood. One of the most common kinase mutations observed in AML patients is internal tandem duplication (ITD) in the juxtamembrane domain (JD) of FMS-like tyrosine kinase (FLT3). The inhibition of FLT3-ITD mutations using FLT3 inhibitors results in the over-expression of FOXO genes in AML patients, leading to upregulation of histone deacetylase (HDAC) and subsequent tumor proliferation and drug resistance due to the inhibition of p53 by over-expressed HDAC. Therefore, there is a need for inhibitors that can target both FLT3-ITD mutations and HDAC. Previous studies have reported the use of theino[2,3-d]pyrimidine-based FLT3-ITD inhibitors. In this study, we have designed molecules that can inhibit both FLT3-ITD mutations and HDAC simultaneously through molecular docking simulation. Synthesis of the designed theino[2,3-d]pyrimidine derivatives is currently in progress, and we have successfully synthesized four compounds. Through comparison of the docking scores of these compounds with actual inhibitory activity, we hope to identify and secure dual-functional inhibitors that can contribute to the development of effective AML treatments.

Poster Presentation : **MEDI.P-408**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

YES1 as a potential therapeutic target in non-small-cell lung cancer

Eunjin Kook[*], **Seoyeon Park, Do-Hee Kim**

Kyonggi University, Korea

Lung cancer is the leading cause of cancer-related mortality worldwide. Non-small cell lung cancer (NSCLC) accounts for about 85% of lung cancer. Drug resistance is the main reason for the failure of chemotherapy in cancer treatments. Recent studies have suggested that overexpression of YES1 promotes cell proliferation, tumorigenesis, and drug resistance in various cancer cells. In this study, we aimed to explore the expression and functional role of YES1 in non-small cell lung cancer (NSCLC) and identify YES1 selective inhibitors. The knockdown of YES1 in NSCLC cells suppressed the expression and phosphorylation of YES1-associated protein 1 (YAP1), leading to the regulation of apoptosis-related proteins. The silencing of YES1 markedly attenuated the migration of NSCLC cells. In addition, expression of YES1, Nrf2, and antioxidant proteins was upregulated in gefitinib-resistant HCC827 (HCC827-Gef) than parent HCC827 NSCLC cells. A new synthetic compound inhibited the proliferation of NSCLC and HCC827-Gef cells. This compound is associated with the downregulation of YES1-mediated signaling pathways in NSCLC cells. Moreover, the combination of gefitinib and synthetic inhibitor showed a synergistic effect on the antiproliferative activity of HCC827-Gef cells to overcome gefitinib resistance. Notably, the knockdown of YES1 blunted the expression of Nrf2-mediated genes. Modulation of YES1 expression/activity may be an attractive therapeutic strategy for the treatment of drug-resistant NSCLC. The identified compound may be a candidate for the development of antitumor agents for NSCLC and drug-resistant NSCLC cells

Poster Presentation : **MEDI.P-409**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Unveiling the mechanism of action of reversible, covalent 3R/4R tau aggregation inhibitors through a molecular dynamics approach.

<u>Lizaveta Gotina</u>, Ae Nim Pae[1,*]

Department of Bio-Medical Science and Technology, University of Science & Technology, Korea
[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

The microtubule-associated protein tau is known to undergo pathological misfolding and subsequent aggregation into oligomers and neurofibrillary tangles, which are directly linked to over 20 diseases (e.g. Alzheimer’s disease (AD), Pick’s disease, etc.) called tauopathies. Despite significant effort over the last decade, only a handful of directly-acting ligands (mostly dye-based molecules or natural products) have been discovered, none of which have yet achieved FDA approval. Tau’s large size, structural polymorphism, and lack of a strictly ordered 3D structure greatly hamper the lead optimization process. The recent major advancement in cryoEM revealed distinct structures of tau filaments and provided the first insights on possible ligand binding sites. Nevertheless, revealing the aggregation inhibitors' mode of action via *in silico* methods remains challenging due to extremely high computational costs and limited structural information.Herein, we create an original, size-optimized, “growing” AD-type tau paired helical protofilament model system and perform 200 ns molecular dynamics (MD) simulations to discover the mechanism of action of a series of in-house designed covalent, reversible tau aggregation inhibitors. Individual evaluation of MD simulations with covalently bound and non-bound ligands reveals the sequence of events leading to tau filament disaggregation. Furthermore, those MD simulations are compared to that of PET tracers (tau-binders, but not tau-disrupting molecules) to highlight the particular binding properties of inhibitor molecules. This work reveals the specific mode of action of a novel class of tau aggregation inhibitors and paves the way to the discovery of tau isoform-specific aggregation inhibitors for treating tauopathies.

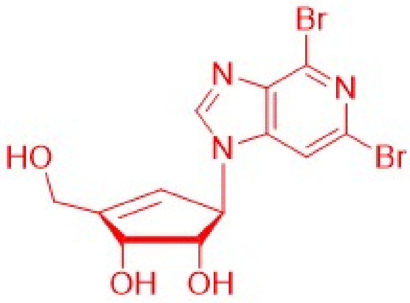
Poster Presentation : **MEDI.P-410**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of 3-deazaneplanocin A Analogs and Their Antiviral Activity against Influenza A Viruses

Se Myeong Choi, Yeon Jin An, Eun Rang Choi, Yong Hun Choi[1], So Jung Kwon, Jong Hyun Cho[*]

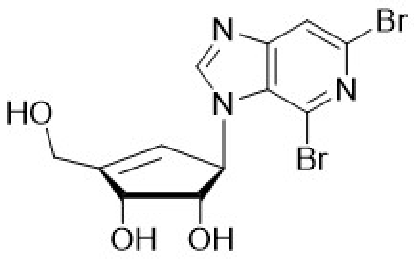
Dong-A University, Korea
[1]*college of Health science, Dong-A University, Korea*

3-Deazaneplanocin A (DENep, 2) analogs showed a broad spectrum of biological activity against some cancers and DNA/RNA viruses as a promising inhibitor of the S-adenosyl-L-homocysteine (SAH) hydrolase and the enhancer of zeste homolog 2 (EZH2). Based on this, many derivatives were synthesized and evaluated, but 6-halogenated DZNep and its analog was not studied as an antiviral agent to date. Thus, N_9 -/N_7 -2,6-dihalo-DZNep and N_7 -6-amino/azido-DZNep analogs were prepared using Mitsunobu reaction of 3-deazapurine derivatives with chiral cyclopentene-1-ol derivatives (22a-b). With a modified procedure of a previous synthetic method, the chiral 22a and 22b were prepared in 50% overall yield from D-ribose. Additionally, 3-deazapurine analogs including 2,6-dibromo-3-deazapurine 30a, 2,6-dichloro-3-deazapurine 30b, 6-azido-3-deazapurine 36. Mitsunobu reaction of 30a-b with 22a afforded a mixture of N_7 -/N_9 -isomer in the ratio of 4:5 and 1:1, respectively. Among prepared DZNep analogs, novel N_9 -2,6-dibromo-3-deazaneplanocin (44a) exhibited the most potent activity (EC_{50} 7. 0 μM) against Flu A (H1N1) with CC_{50} >100 in vitro. Unexpectedly, N_7 -6-azido-3-deazaneplanocin (46) displayed EC_{50} 22.5 μM, and 25.3 μM against Flu A (H1N1) and (H3N2) with CC_{50} >100 , respectively. The other 3-DZNep analogs showed no significant antiviral potency against Flu A and B in vitro and against dengue virus-2 replicon. Currently, N9 -2,6-dibromo-3-deazaneplanocin (44a) was found as a new hit compound for Flu A (H1N1).



N_9-Isomer

vs



N_7-Isomer

$EC_{50} = 7.6\ \mu M$ (Flu A, H1N1)
$CC_{50} > 100\ \mu M$

$EC_{50} > 100\ \mu M$ (Flu A, H1N1)
$CC_{50} > 100\ \mu M$

Poster Presentation : **MEDI.P-411**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and biological evaluation of new *β*-D-N^4-hydroxycytidine analogs against SARS-CoV-2, influenza viruses and DENV-2

Yeon Jin An, Se Myeong Choi, Eun Rang Choi, Ji Yeon Yang[1], A Young Jung[2], Jong Hyun Cho[*]

Dong-A University, Korea
[1] *college of Health science, Dong-A University, Korea*
[2] *Health science, Dong-A University, Korea*

Drug repurposing approach was applied to find a potent antiviral agent against RNA viruses such as SARS-CoV-2, influenza viruses and dengue virus with a concise strategy of small change in parent molecular structure. For this purpose, *β*-D-N^4-hydroxycytidine (NHC) with a broad spectrum of antiviral activity was chosen as the parent molecule. Among the prepared NHC analogs from uridine, *β*-D-N^4-O-isobutyrylcytidine showed potent activity against SARS-CoV-2 (EC_{50} 3.50 μM), Flu A (H1N1) (EC_{50} 5.80 μM), Flu A (H3N2) (EC_{50} 7.30 μM), Flu B (EC_{50} 3.40 μM) and DENV-2 (EC_{50} 3.95 μM) in vitro. Furthermore, its potency against SARS-CoV-2 was >5-fold, 3.4-fold, and 3-fold compared to that of NHC, MK-4482, and remdesivir (RDV) in vitro, respectively. Ultimately, *β*-D-N^4-O-isobutyrylcytidine was expected to be a potent inhibitor toward RNA viruses as a viral mutagenic agent like MK-4482.

Poster Presentation : **MEDI.P-412**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Optimization strategy of a novel N-((6-(substituted-amino)-2-methyl-2H-chromen-2-yl)methyl)-N-methylbenzenesulfonamide derivatives as 5-lipoxygenase inhibitors based on molecular hybridization

Young-Chang Kim, Hyeong Hee Kim, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

5-Lipoxygenase (5-LO) is one of the significant drug targets for the treatment of various inflammatory diseases. Herein, we designed, optimized, and synthesized novel N-((6-(substituted-amino)-2-methyl-2H-chromen-2-yl)methyl)-N-methylbenzenesulfonamide derivatives as potential 5-LO inhibitors. In this work, particularly, we applied concept of 'Molecular Hybridization' for structural optimization. Among the synthesized compounds, 10a, 10b, and 10g exhibited inhibitory activity toward 5-LO according to the in vitro studies including enzyme activity assay (≥ 78% inhibition at 1 μM) and cell-based assay (≥ 72% inhibition at 1 μM). 10b was selected for further in vivo evaluation using an arachidonic acid-induced ear edema mouse model. Oral administration of 10b successfully suppressed ear edema and myeloperoxidase activity (MPO activity). Molecular docking studies suggest an allosteric binding mode between 5-LO and compound 10b.

Poster Presentation : **MEDI.P-413**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enantioselective synthesis of an N-methylated cryptophycin analogue with a facile approach to unit A

Young Chae Kim, Hyejin Ahn[1], Jisu Do[1], Sang Jeon Chung[2,*]

Sungkyunkwan University, United States
[1]*Sungkyunkwan University, Korea*
[2]*College of Pharmacy, SungKyunKwan University, Korea*

Antibody-drug conjugates (ADC) are a class of novel anticancer therapeutics which employ the properties of an antibody to target cancer cells while minimizing off-target effects. The cytotoxic element of an ADC comes from a payload which is often too potent to be used on its own. Cryptophycin is a class of cytotoxic molecules that shows promise as a potential ADC payload. Using published structure-activity relationship (SAR) studies, we designed an analogue of cryptophycin that features an N-methylated unit B which can be used as a linker attachment site in an ADC while maintaining cytotoxicity. Further, we also designed a shorter, easier synthetic scheme for unit A, which has historically been the largest and most difficult to synthesize.

Poster Presentation : **MEDI.P-414**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Covalent-Handled Molecular Glue Degrader for Anaplastic Lymphoma Kinase(ALK)

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[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Approximately 3%-5% of patients with non-small cell lung cancer (NSCLC) carry anaplastic lymphoma kinase (ALK) gene fusions and benefit greatly from ALK-targeted therapy. Potent ALK inhibitors, including crizotinib, alectinib, ceritinib, and brigatinib, have demonstrated significant efficacy against ALK-mutated NSCLC. Targeted protein degradation using molecular glues is a promising approach to eliminate undruggable disease-causing proteins. In this study, we aimed to identify a transposable chemical handle that could convert protein-targeting ligands into molecular degraders that target ALK. In this experiment, we identified a degrader that efficiently targets cysteine 32 in the RING family E3 ubiquitin ligase RNF126, leading to the degradation of ALK proteins. The developed ALK-targeted molecular glues effectively degraded oncogenic ALK driver proteins.

Poster Presentation : **MEDI.P-415**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Design and synthesis of a potential building block for diverse mitochondria-targeted theranostics

Kyeongyang Lee, Ji Young Choi, Byung Chul Lee[1,*]

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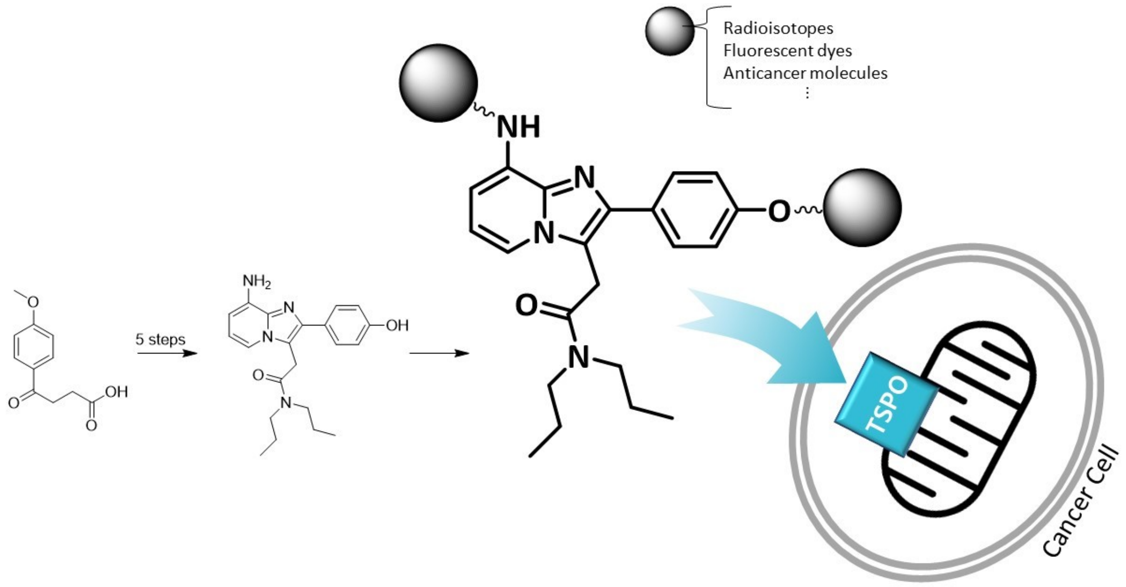
The translocator protein 18 kDa (TSPO) is overexpressed in many cancers and has been recognized as a potential target for cancer theranostics due to its localization in the mitochondrial membrane. Incorporating a TSPO-binding molecule as a building block can improve the selectivity of theranostics into cancer mitochondria. Specifically, the use of a TSPO-targeting building block in conjugation with a theranostic agent could provide the preferential accumulation in cancer mitochondria, ultimately improving the efficiency of theranostics. We designed the novel TSPO-targeting building block readily to introduce radioisotopes, fluorescent dyes, and anticancer molecules without being interrupted by cancer mitochondria-targeting. The novel TSPO-targeting building block consists of hydroxy and amino groups, including TSPO-binding moiety. The TSPO-binding building block was prepared under the known method of imidazopyridine-based TSPO ligands, but synthetic limitations such as low chemical yield and purity did require optimization in detail. In enhanced results, the yield of the imidazopyridine formation step was increased 7-fold compared to known conditions by optimizing the solvent and temperature. The use of a non-metal reducing agent provided the pure 8-amino imidazopyridine derivative without interfering with residual metal in the product. Finally, the novel TSPO-targeting building block was synthesized in 5 steps from 3-(4-methoxybenzoyl)propionic acid and showed high TSPO binding affinity (Ki = 158 nM). The potential TSPO-targeting fluorescent probes and radiotracers were usefully prepared from the novel building block. Therefore, we anticipate that this potential building block could be exploited as diverse strategies for developing mitochondria-targeted theranostics.


Radioisotopes
Fluorescent dyes
Anticancer molecules
5 steps
TSPO
Cancer Cell

Poster Presentation : **MEDI.P-416**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Thiirane-mediated Chemical Tools for S-sulfhydration

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[3]*Chemistry, Gangneung-Wonju National University, Korea*

Reactive sulfur species (RSS) are biologically important molecules. Among them, persulfides (RSSH) play critical regulatory functions in redox cell signaling. However, persulfides are unstable and difficult to measure the concentration of their formation directly. Therefore, intelligent chemical tools are needed to efficiently generate persulfides in situ to investigate the effects of persulfides in biological systems. Here, we report the synthesis of thiiranes which generate persulfide species by reacting with biological thiols and give a fluorescence signal corresponding to the concentration of persulfides. With this unique approach of directly generating persulfides, we also showed efficient S-sulfhydration of a protein. This new approach should allow a complement to current chemical tools for the investigation of persulfides in living systems.

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Poster Presentation : **MEDI.P-417**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis and Evaluation of Polysulfide-engineered Silicon Nanoparticles for Hydrogen sulfide Donors

Yerim Lee, Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea

Hydrogen sulfide (H_2S) has been recognized as a gaseous signaling molecule involved in regulating many physiological and pathological processes. However, small molecules that release H_2S have been developed as it is difficult to handle the gas directly. Here we report polysulfide-engineered silica-based nanoparticles that release H_2S by interactions with intracellular thiols. We designed and synthesized polysulfide-coated nanoparticles engineered with the reactions between pyridyl disulfides and tralkyl silanethiols in aqueous media. We investigated the synthesis efficacy and H_2S release ability of the nanoparticles. In addition, we intend to functionalize the nanoparticle surface containing the medicinal effect of H_2S and apply it to various disease models.

Poster Presentation : **MEDI.P-418**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Design and Synthesis of Novel Sphingosine-1-Phosphate Receptor 1 (S1PR1) Agonists for the Treatment of Multiple Sclerosis

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*

Multiple sclerosis (MS) is the chronic neuroimmune disease that affects the central nervous system, including the brain, spinal cord, and optic nerve. The pathological features of MS are extensive, including movement disorders, vision, eye pain, sensory loss, memory loss, and depression. Multiple sclerosis results from demyelination of myelin sheaths in the central nervous system. To prevent demyelination, this study focused on preventing T-cell from leaving lymph nodes by inhibiting the S1PR1 present on T-cell. We found compounds KDS8109 with superior efficacies by changing the central heterocore of previous isoxazoline derivatives to 1,2,4-oxadiazole derivatives. Although some isoxazoline derivatives also have a few nanomolar EC50 value in β -arrestin assay and internalization assay, KDS8109 showed better efficacies in vitro experiments. (EC50 = 2.16 nM for internalization, EC50 = 5.57 nM for β-arrestin recruitment). Additional experiments were performed to validate the in vivo experiments. It was confirmed that the number of lymphocytes effectively decreased in the mice treated with KDS8109 and then returned to the basal level. In addition, it was confirmed that in Experimental Autoimmune Encephalomyelitis (EAE) mouse immunized with MOG protein and P.T protein, compound KDS8109 treatment compared to vehicle inhibited the increase in clinical score.

Poster Presentation : **MEDI.P-419**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Sphingosine-1-phosphate receptor 1 Agonists for Treatment of Multiple Sclerosis

Jaehwan Kim, Ki Duk Park[*]

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

Multiple sclerosis (MS) is a neurodegenerative disease that affects the central nervous system (CNS) by autoreactive lymphocytes that attack the myelin sheath. Approximately 80% of MS patients are initially diagnosed with relapsing-remitting MS (RRMS) characterized by repeated periods of increased neurological symptoms (relapsing) and partial recovery (remitting). Relapse is associated with epitope spreading during myelin destruction and remissions is associated with a temporary loss of immune cells in the CNS. Therefore, reducing the entry of lymphocytes into the CNS is an effective strategy for treating MS. Sphingosine-1-phosphate receptor 1 (S1P1), a G-protein-coupled receptor, plays an important role in promoting the egress of lymphocytes from lymphoid organs into the blood circulation. Activated S1P1 by ligand binding triggers the lymphocyte egress through G-protein signaling, but some agonists block G-protein signaling by recruiting β-arrestin. Desensitized S1P1 is internalized into cells and degraded, resulting in sequestration of lymphocytes into lymphoid organs. In this study, we developed new S1P1 agonists that showed better efficacy than FDA-approved drugs fingolimod and ozanimod in in vitro tests. To evaluate in vivo efficacy of the best compound, KDS8024, we confirmed the peripheral lymphocyte reduction and the therapeutic effect in experimental autoimmune encephalomyelitis (EAE), an animal model of MS.

Poster Presentation : **MEDI.P-420**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of 3H-[1,2,3]triazolo[4,5-d]pyrimidine by using microwave to find out optimization strategy

Dahee Boo, Sanghyun Lee, Seung Beom Cheon, Young Dae Gong[1,*]

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

Furin is involved in numerous biological processes, such as viral propagation, bacterial toxin activation, cancer, and metastasis. Triazolopyrimidine is one of the – isostere of purine. According to the previous research, [1,2,4]triazolo[1,5-c]pyrimidine showed good association between PfDHODH inhibition and parasite toxicity. This study has identified the first nanomolar PfDHODH inhibitor with potent antimalarial activity in whole cells. Also in another research, 1,2,4-Triazolo[1,5-a]Pyrimidine which are tested for their in vitro antibacterial and antifungal activities showed that comparable results with those of ampicillin and fluconazole reference drugs.So we slightly substitute our structure from [1,2,4]triazolo[1,5-c]pyrimidine to 3H-[1,2,3]triazolo[4,5-d]pyrimidine. We tried to optimize the best situation by using microwave in 3 steps. By optimization, we can reduce time and obtain a higher yield. Also, 3H-[1,2,3]triazolo[4,5-d]pyrimidine is expected to have similar potentialities of [1,2,4]triazolo[1,5-c]pyrimidine as mentioned earlier.

Poster Presentation : **MEDI.P-421**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of human tribbles homolog 2 pseudo serine/threonine kinase (TRIB2) inhibitors to overcome triple negative breast cancer (TNBC)

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

Triple-Negative Breast Cancer (TNBC) is one of the most challenging breast cancers to overcome. In general, aiming at three well-validated targets, such as estrogen receptor (ER), progesterone receptor (PR), and human epidermal growth factor receptor 2 (HER2), could be typical strategies to discover small molecule drugs for the treatment of breast cancers. In contrast, TNBC lacks these three receptors. In addition, TNBC has a poor prognosis due to few treatment options. Nevertheless, TNBC is composed of more than 10 % of total breast cancer patients. Tribbles homolog 2 (TRIB2) is a pseudo serine/threonine kinase without a catalytic function expressing multifunctional oncogenic roles. It has been known that TRIB2 is involved in survival and drug resistance in solid and hematologic cancers. TRIB2 is considered a direct target of Notch1, which is related to a hallmark for TNBC. Thus, inhibition of TRIB2 could be an effective strategy to overcome TNBC. With a view to developing an anti-TNBC drug candidate, we launched our campaign to discover TRIB2 inhibitors by high-throughput screening of a virtual liabrary from the Korea Chemical Bank. In this work, we will discuss our strategies to discover TRIB2 inhibitors. In addition, biological data profiles of some of selected TRIB2 inhibitors will be presented, such as TRIB2 enzyme activity and in vitro anti-cancer activity against TNBC cell line MDA-MB 231.

Poster Presentation : **MEDI.P-422**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Design and synthesis of small molecule JAK1 Inhibitors for the treatment of autoimmune diseases

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

AbstractThe Janus kinase (JAK) is one of the most popular drug targets for autoimmune diseases. Indeed, there are several approved JAK inhibitors, such as tofacitinib, baricitinib, and ruxolitinib. Although JAK is well-validated target for autoimmune diseases, selectivity was a major issue to consider. In this context, JAK1 selective inhibitors have obtained tremendous attention. Filgotinib is considered to be a promising JAK1 selective inhibitor undergoing diverse clinical trials. We opted to discover JAK1 selective inhibitors by modifying the structure of filgotinib. Our design strategies and synthetic approaches will be discussed. Moreover, biological activities and ADME/Tox profile of some of selected compounds will be presented.

Poster Presentation : **MEDI.P-423**
Medicinal Chemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Discovery of Novel Mixed-Lineage Kinase 3 (MLK3) Inhibitors as Anti-Ovarian Cancer Agents

Vineetkumar bapusaheb Patil, Pilho Kim[1,*], Kyoung Ok Hong[2]

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[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*
[2]*R&D center, Genesen Co., Ltd., Korea*

Mixed-lineage kinase 3 (MLK3) belongs to mitogen-activated protein 3 kinase kinases (MAP3K) which are involved in various MAP signaling cascades, such as c-Jun N-terminal kinase (JNK)/Stress-activated protein kinase (SAPK), Extracellular-signaling regulated kinase (ERK), and P38 NAPK. Due to its role in various signaling pathways, MLK3 is implicated in proliferation, differentiation, migration, invasion, and apoptosis of tumors including breast, cervical, colorectal, gastric, prostate, and ovarian cancers. In addition to cancers, MLK3 is also involved in certain neurocognitive and neurodegenerative diseases like HAND and Parkinson’s diseases. Ovarian cancer (OC) is a most common gynecologic malignancy which is responsible for at least 20% of all cancer-related deaths in women. In addition, there is no effective treatment to cure OC with no or minimal adverse effects. Studies on OC cells have revealed that the presence of higher levels of MLK3 as well as abnormal regulation of MLK3, when compared to non-tumorigenic cells. It has been known that matrix metalloproteinases (MMP-1 to 9) are regulated by JNK and ERK pathways which in turn are responsible for the progression of OC. Studies have shown that MMP expression level is related to the invasion of cancer cells, thus, overexpression of MMP3 could cause severe tumor progression. Furthermore, the MMP levels are determined by MLK3 activity and silencing of MLK3 by siRNA lowers the MMP expression, whereas MLK3 overexpression leads to increased MMP levels. Hence, these results suggest that targeting MLK3 protein could be an effective strategy for the treatment of OC. Only a few inhibitors have been reported, such as CEP-1347 for Parkinson’s disease and URMC-099 for HIV-associated dementia. As our continuous efforts on anti-cancer drug discovery, we have designed and synthesized MLK3 inhibitors targeting OC. Biological activities and druggability data of selected compounds will be presented.

Poster Presentation : **MEDI.P-424**

Medicinal Chemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nrf2 activator exert anti-inflammatory effects in DNCB-induced Atopic Dermititis-like mouse model

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Korea Institute of Science and Technology, Korea

[1] *Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Atopic Dermatitis (AD) is a chronic inflammatory skin disease characterized by itching, dryness, hemorrhage and eczematous lesions. The nuclear factor E2-related factor 2 (Nrf2) is a crucial regulator of cellular defense mechanism against oxidative stress by inducing the expression of antioxidant and anti-inflammatory genes. In this study, we designed and developed Nrf2 activators to maximize its antioxidant and anti-inflammatory activity to treat AD inflammatory skin disease. Among the compounds, KDS10063 exhibited the most prominent Nrf2 activating efficacy. Treatment with KDS10063 significantly increased Nrf2 protein level and induced Nrf2-dependent antioxidant enzymes at protein and mRNA level in HaCaT keratinocyte cells. KDS10063 dose-dependently reduced the expression of proinflammatory cytokines IL-6 and TNF-α also at protein and mRNA level in TNF-α/IFN-γ-stimulated HaCaT cells. As macrophage cells play an key role in inflammatory response, we confirmed that KDS10063 remarkably inhibited Nitric Oxide (NO) production and proinflammatory cytokines in LPS-stimulated RAW264.7 macrophage cells. Additionally, we found that KDS10063 reduced the skin barrier damage, increase in lymph node weight and also serum IgE level in 2,4-dinitrochlorobenzene (DNCB)-induced AD-like skin inflammation mouse model. Taken together, our study suggest that KDS10063 could be a potential treatment for atopic dermatitis inflammatory disease.

Poster Presentation : **MAT.P-282**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

2D-Pt Nanodendrites with Manipulated Crystal Facets: Intimately Coupled Electrocatalytic Heterointerface for Hydrogen Evolution Reaction

Yu-Rim Hong, In Su Lee*

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

Despite notable signs of progress in Pt-catalyzed alkaline hydrogen evolution reaction (HER) via hybridizing with oxophilic metal-hydroxide surface, maximization of Pt's reactivity alongside operational stability are still unsatisfactory due to the lack of well-designed and optimized interface structure. Herein, by devising atomically-flat 2D-Pt nanodendrite (2D-PtND) under the deployment of our strategized 2D-nanospace-confined synthesis, it offers all sorts of Pt features to tackle the poor-and-insufficient interfacial impacts in HER catalysis by simultaneously realizing an area-maximized and firmly-bound lateral heterointerface with NiFe-layered double hydroxide (LDH). In particular, the accompanied well-oriented (110) facet exposure of Pt has recognized a massive electronic interplay that certainly bestows strong LDH-binding. As a result, the charge-relocated interfacial bonds in 2D-PtND/LDH acted favorably in accelerating the hydrogen generation steps and reaching about one of the highest reported Pt-mass-activity improvements (~11.2 times greater than 20 wt% Pt/C) with a substantially enhanced long-term operational stability. This work uncovers the importance of the shape and facet of Pt in feasible heterointerface creation to strengthen the catalytic synergies for efficient hydrogen production.

Poster Presentation : **MAT.P-283**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Defect-rich holey 2D ruthenium phosphide nanosheets for enhanced hydrogen evolution electrocatalysis

Xiaoyan Jin, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

The exploration of efficient electrocatalysts has evoked intense scientific efforts because of crucial role of electrocatalytic reactions in renewable energy technologies. Here we report a novel methodology to explore high-performance electrocatalysts for hydrogen evolution reaction (HER) via the formation of defective holey nanosheet with enhanced hydrogen accumulation capability. The efficient 2D nanostructured electrocatalysts of subnanometer-thick holey Ru_2P nanosheets with plenty of crystal defects could be synthesized by phosphidation of monolayered RuO_2 nanosheets. In comparison with non-holey Ru_2P nanoparticles, holey Ru_2P nanosheet delivered much better HER activity with very small overpotentials of 17 and 26 mV for acidic and alkaline electrolytes, respectively. Thus, they are among the best-performing Ru-P-based HER catalysts reported thus far. Systematic in situ spectroscopic investigations underscored that holey nanosheet morphology enhanced the adsorption of proton/water and the accumulation of adsorbed hydrogen, leading to the increased contribution of Volmer-Tafel mechanism to the HER activity of ultrathin holey Ru_2P nanosheets.

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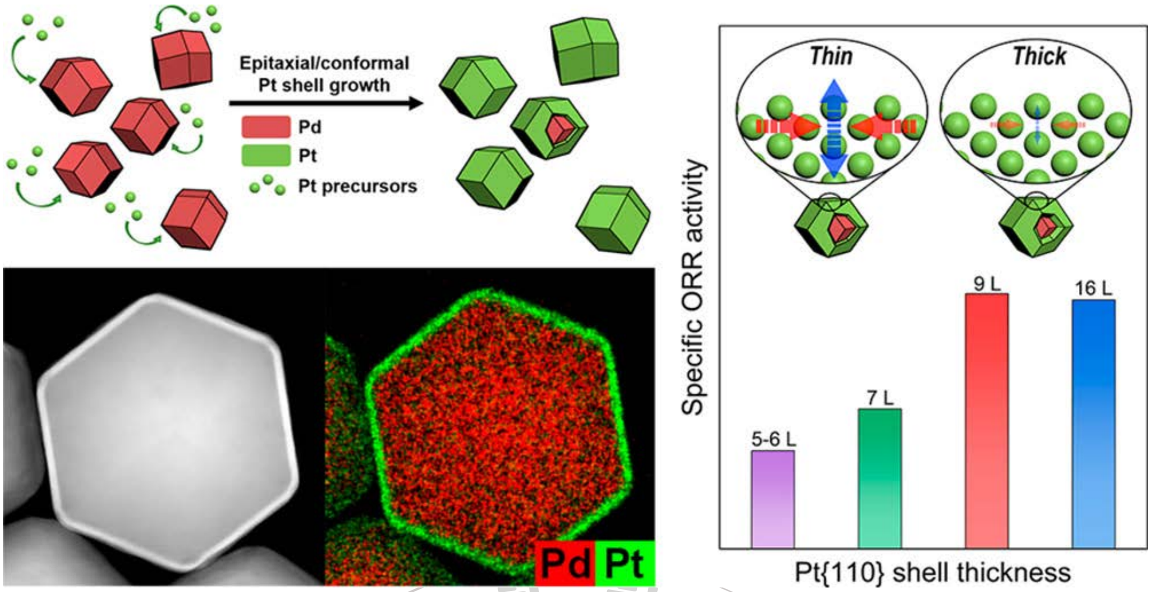
Poster Presentation : **MAT.P-284**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Exploring the relationship between strain and oxygen reduction reaction activity on Pt{110} facets

Hochan Ahn, Sang Woo Han[*]

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

We have developed a synthesis method of rhombic dodecahedral Pd@Pt core–shell nanocrystals bound exclusively by {110} facets with controlled numbers of Pt atomic layers to study the surface strain–catalytic activity relationship of Pt{110} facets. Through control over growth kinetics, the epitaxial and conformal overgrowth of Pt shells on the {110} facets of rhombic dodecahedral Pd nanocrystals could be achieved. Notably, the electrocatalytic activity of the Pd@Pt nanocrystals toward oxygen reduction reaction decreased as their Pt shells became thinner and thus more in-plane compressive surface strain was applied, which is in sharp contrast to previous reports on Pt-based catalysts. Density functional theory calculations revealed that the characteristic strain–activity relationship of Pt{110} facets is the result of the counteraction of out-of-plane surface strain against the applied in-plane surface strain, which can effectively impose a tensile environment on the surface atoms of the Pd@Pt nanocrystals under the compressive in-plane strain


Epitaxial/conformal
Pt shell growth
Pd
Pt
Pt precursors
Pd
Pt
Thin
Thick
Specific ORR activity
5-6 L
7 L
9 L
16 L
Pt{110} shell thickness

Poster Presentation : **MAT.P-285**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Active Site Identification for H_2O_2 Electrosynthesis by Molecular Functionalization of Carbon Nanotubes

Yongjin Jung, Yesol Lee, Young Jin Sa*

Department of Chemistry, Kwangwoon University, Korea

The electrochemical production of H_2O_2 via the two-electron oxygen reduction reaction ($2e^-$ ORR) has recently attracted attention as a promising alternative to the current anthraquinone process. Identification of active sites in O-doped carbon materials, which exhibit high activities and selectivities for the $2e^-$ ORR, is important for understanding the selective electrocatalytic process and achieving the rational design of active electrocatalysts. However, this is impeded by the heterogeneous distribution of various active sites on these catalysts. In this study, we exploited the molecular functionalization approach to implant anthraquinone, benzoic acid, and phenol groups on carbon nanotubes and systematically compared the electrocatalytic activities and selectivities of these functional groups. Among these oxygen functional groups, the anthraquinone group showed the highest surface-area-normalized and active-site-normalized activities.

Poster Presentation : **MAT.P-286**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Stability improvement of bioactive organic molecules in the interlayer space of layered rare earth hydroxides

Myeongjin Kang, **Song-ho Byeon**[1,*]

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[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

The encapsulation of organic guest molecules into inorganic hosts has been extensively investigated to synergistically improve the physicochemical properties of guest and host materials. For instance, bioactive organic molecules, which are easily deteriorated by heat, oxygen, light, or condition of biosystem, could efficiently perform biologically important functions when they are effectively protected from such degradations. Recently developed layered rare earth hydroxides (LRHs) have attracted much interest as a host system able to give an environment for safe storage and effective delivery of such guest molecules. In this work, we synthesized LRHs intercalated with some biologically important molecules in their interlayer galleries and evaluated the improvement of stabilities in the ambient environment or under simulated special conditions. Activator ions such as Eu^{3+} and Tb^{3} were doped to monitor the sensitization effect by interlayer organic molecules and to demonstrate the capability as a fluorescence probe.

Poster Presentation : **MAT.P-287**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

LRHs for room temperature synthesis of RVO4 (R = rare earths) nanoparticles and fabrication of their heterostructured composite films

Yoonjae Choi, Song-ho Byeon[1,*]

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[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

A new strategy was developed for the synthesis and the size control of RVO4 (RE = rare earths) nanoparticles using LRHs (layered rare earth hydroxides) as precursors in aqueous solutions. For instance, GdVO4:Eu3+ nanoparticles were synthesized using the layered gadolinium hydroxychloride doped with Eu3+ (LGdH:Eu) as a precursor in an aqueous metavanadate solution. No heating process was required in this procedure but the particle size was controllable by adjusting the solution pH or salt. A representative up-converting YVO4:20%Yb3+,0.4%Ho3+ particle was also synthesized using LYH:Yb,Ho as a precursor in an aqueous orthovanadate solution at room temperature. As the prepared elliptical shaped YVO4:Yb,Ho particles maintained high dispersibilty even after annealing at 700℃ in aqueous PVA solutions, they could be exploited for the fabrication of highly efficient up-converter YVO4:Yb,Ho/PVA composite films. Furthermore, a heterostructured photoluminescence 'turn-off' film was fabricated using vertically oriented LYH:Eu nanosheets as a partial sacrificial layer for isolated YVO4:Eu3+ nanophosphor layers. In situ immobilized YVO4:Eu3+ nanophosphor film was applied for the convenient detection and removal of Cu2+ ions with excellent sensitivity and recyclability.

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Poster Presentation : **MAT.P-288**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Intrinsic Activity and Reaction Selectivity toward Oxygen Reduction Reaction on Metal Phthalocyanines

Yesol Lee, Young Jin Sa[*]

Department of Chemistry, Kwangwoon University, Korea

Atomically dispersed transition metal catalysts on N-doped carbons (M–N/C catalysts) are promising alternatives to precious metal catalysts for electrochemical oxygen reduction reaction (ORR). ORR can take multiple reaction pathways depending on the catalysts, where 2-electron ORR ($2e^-$ ORR; $O_2 + 2H^+ + 2e^- \rightarrow H_2O_2$) and 4-electron ORR ($4e^-$ ORR; $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$) are important reactions for H_2O_2 electrosynthesis and fuel cells, respectively. Understanding the structure–activity–selectivity relationship provides design strategies for developing highly active and selective M–N/C-based ORR electrocatalysts, which, however, is impeded by the formation of various active sites in typical pyrolyzed M–N/C catalysts. In this work, we prepared M–N/C catalysts with multiple metal centers, yet with an identical coordination environment using metal phthalocyanine molecules supported on carbon nanotube (MPc/CNT). The trends of intrinsic catalytic activity and selectivity toward the ORR were investigated in neutral and alkaline electrolytes to reveal the effect of metals in the MPc/CNT catalysts. CoPc/CNT shows the highest $2e^-$ ORR activity among the MPc/CNT catalysts. Meanwhile, FePc/CNT and MnPc/CNT are highly active for the $4e^-$ ORR, where FePc/CNT and MnPc/CNT catalyze the reaction in different reaction pathways: direct $4e^-$ ORR for FePc/CNT, and $2e^-$ ORR and subsequent H_2O_2 reduction ($2e^- \times 2e^-$ ORR) for MnPc/CNT.

Poster Presentation : **MAT.P-289**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Carbon Nanotube– Electrolyte Interface Modification by Ceria Nanoparticles for Efficient H_2O_2 Electrosynthesis

Sohee Kim, Young Jin Sa*

Department of Chemistry, Kwangwoon University, Korea

The electrochemical production of H_2O_2 by 2-electron oxygen reduction reaction ($2e^-$ ORR; $O_2 + 2H^+ + 2e^- \rightarrow H_2O_2$) has attracted attention as an alternative to the anthraquinone oxidation process that has environmental and cost issues. Active and selective electrocatalysts for the $2e^-$ ORR are critical for the efficient H_2O_2 electrosynthesis; otherwise, the parasitic 4-electron ORR ($4e^-$ ORR; $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$) occurs. Carbon-based nanomaterials have been actively investigated owing to chemical tunability and high efficiency for $2e^-$ ORR; however, they have high $2e^-$ ORR activity only in alkaline solutions in which H_2O_2 is easily decomposed. In this work, we prepared ceria nanoparticles on carbon nanotubes (CeO_2/CNT) to investigate the role of the supported ceria, which has shown low activity in many electrocatalytic reactions. The CeO_2/CNT catalysts exhibited better $2e^-$ ORR activity than bare CNT in a neutral electrolyte. The activity improvement factor was similar regardless of the ceria contents, presumably suggesting the CNT–electrolyte interface modification by the ceria rather than direct participation in the electrocatalysis.

Poster Presentation : **MAT.P-290**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Magnetic devourers with hydrophilic and hydrophobic tentacles for fast and easy removal of microplastics

Su Hyeon Son, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Microplastics, a type of pollutants, have become a matter of widespread concern owing to their potential environmental and health problems. Microplastics that are found in oceans, rivers, soil, and even air, can be further oxidized or broken into smaller nanoplastics by sunlight, collisions, and friction. The nanoplastics have a greater risk to human beings and environment. We report amphiprotic magnetic scavengers for fast and easy elimination of hydrophilic and hydrophobic microplastics.

Poster Presentation : **MAT.P-291**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Solar-induced pure water-generating devices with light-harvesting and collection systems

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[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Shortage and pollution of water have accelerated the study on solar-induced water evaporation and purification using inexhaustible solar energy. For efficient water evaporation and purification, high water-absorbing abilities, excellent photothermal properties, and high specific surface areas are essential. However, the development of absorbent/evaporators with excellent photothermal and water-absorbing abilities is still changing. In this study, pine-needlelike structured absorbent/evaporators with high specific surface areas were formed by bottom-up and sacrificial approaches.

Poster Presentation : **MAT.P-292**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Lithium ionic conductor with new type of crystal structure

Jihun Roh, **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*

Discovering a new ionic conductor is a crucial but challenging task due to complicated material designs related to crystal structure and ionic conductivity. In this report, we present new type of lithium ionic conductor. The crystal structure of thio-germanate, which has been remained unclear, was determined by capillary powder X-ray diffraction for the first time. It showed the structure type of wurtzite ZnS, with the distorted hexagonal close packed of sulfur anions in the direction of c–axis. All the cations in the unit cell occupied in half of tetrahedral interstices except one lithium, which placed on the middle of the interplanar in trigonal-bipyrimidal site. The material displayed ionic conductivity of 2.2×10−6 S cm−1 at 473 K, and bond valence energy landscape (BVEL) calculation revealed three-dimensional lithium diffusion pathways in the unit cell. These results suggest that this new thio-germanate may serve as an lithium ionic conductor, with precise synthetic design.

Poster Presentation : **MAT.P-293**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Crystal structures and ionic conductivities of $Li_{3-x}Al_{1-x}Si_{1+x}O_5$ (x = 0-0.10)

Songhyeon Kim, **Young-il Kim***

Department of Chemistry, Yeungnam University, Korea

Lithium aluminosilicate Li_3AlSiO_5 crystallizes in a wurtzite-like structure where the LiO_4, AlO_4, and SiO_4 tetrahedra are ordered perfectly. The high Li population in Li_3AlSiO_5 allows for the 3-dimensional corner-shared linkage of LiO_4 tetrahedra, in which each tetrahedron is surrounded by four octahedral voids. Such a structural aspect is closely relevant to ionic conductivity. In this study, we prepared Li_3AlSiO_5 and $Li_{3-x}Al_{1-x}Si_{1+x}O_5$ (x = 0.02, 0.05, 0.10) by the citrate sol-gel route, and carried out neutron diffraction, magic angle spinning solid-state nuclear magnetic resonance spectroscopy (^{7}Li, ^{27}Al, ^{29}Si), and impedance spectroscopy. Composition-dependent evolutions of lattice constants and ionic conductivity are to be presented, and the Li vacancy sites in $Li_{3-x}Al_{1-x}Si_{1+x}O_5$ will be discussed based on the neutron Rietveld refinement.

Poster Presentation : **MAT.P-294**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A pervaporation process for the dehydration and purification of chemicals with graphene oxide membrane

Byeongho Lee, Choonsoo Kim*

Department of Environmental Engineering, Kongju National University, Korea

The membrane separation for the dehydration and purification of chemicals called pervaporation (or pervaporative separation), has been widely studied as a feasible alternative to the traditional distillation method for the separation process. The pervaporation (feed: liquid phase) and vapor permeation (feed: vapor phase) are membrane-based processes for the selective separation of mixtures of liquids or vapor by partial vaporization through a non-porous or porous membrane that acts as a selective barrier between feed and permeate. In this research, it exhibits that the graphene oxide (GO) membrane enables the separation of water-alcohol binary vapor through the vapor permeation process. GO membrane allows selective permeation of only water through the membrane due to its hydrophilicity so it is demonstrated the GO membrane is excellent as the next-generation pervaporation membrane for the purification of alcohols.

Poster Presentation : **MAT.P-295**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Zr-based UiO-67 metal-organic framework functionalized with aminosilanes: Selective adsorbent for CO_2 capture at low pressure

Ha-Young Nam

Kyungpook National University, Korea

Effective CO_2 removal 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-296**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Porous carbon converted from a non-porous metal-organic framework for adsorptive removal of sulfanilamide and chloroxylenol from water

Jeongbin Lee

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Three isomeric metal-organic frameworks (MOFs) such as MAF-5, -6, and -32 (with the same composition of [Zn(2-ethylimidazole)$_2$]) were carbonized and, for the first time, activated further with KOH to prepare highly porous MOF-derived carbons (MDCs). Importantly, MDC-32 derived from non-porous MAF-32 had the highest porosity among the three MDCs although it has the lowest porosity when no KOH activation was done. Adsorption of sulfanilamide and chloroxylenol from water was investigated with the MDCs. Among the MDCs, MDC-32 showed the best adsorptive performance for sulfanilamide and chloroxylenol. Moreover, MDC-32, had the highest adsorption capacity (256 mg/g) for removing sulfanilamide from water, compared with any adsorbent reported so far. Based on the observed adsorption and properties of the adsorbate and adsorbent, $\pi-\pi$ and hydrogen bonding interactions, with a slight contribution of repulsive electrostatic interaction, could be suggested as the mechanism for the sulfanilamide adsorption over the MDC-32. Moreover, the MDC-32 could be recycled easily for up to four cycles. It could be suggested that non-porous MOFs can be a good precursor for highly porous MDCs, if activated well using KOH, for example. Finally, MAF-32-derived carbon, MDC-32, might be suggested as a plausible adsorbent to eliminate organics such as sulfanilamide and chloroxylenol from water.

Poster Presentation : **MAT.P-297**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Metal–Semiconductor–Metal Ternary Heteronanocrystals with Multiple Plasmonic Effects for Efficient Photocatalytic Hydrogen Evolution

Yonghyeon Kim, **Sang Woo Han***

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

Regarding the design of high-performance solar energy conversion platforms, heteronanostructured photocatalysts consisting of plasmonic metals and semiconductors are of particular interest due to their capability for the conversion of solar to plasmon energy that can accelerate the formation of charge carriers. Here, we introduce ternary heteronanocrystals composed of two different plasmonic metal nanocrystals (hexoctahedral Au and spherical Ag nanocrystals) and a semiconductor (Cu2O). The site-selective overgrowth of Cu2O on the high-curvature vertices of hexoctahedral Au nanocrystals and the subsequent deposition of spherical Ag nanocrystals on the Cu2O surface could realize the formation of Au–Cu2O–Ag ternary heteronanocrystals with a precisely controlled configuration. The synthesized ternary heteronanocrystals exhibited enhanced photocatalytic H2 evolution performance under a wide range of visible-light irradiation compared to binary and monomeric counterparts. The improved photocatalytic function of the ternary heteronanocrystals can be attributed to the combination of the two different plasmonic metal nanocrystals having distinct plasmonic properties with the semiconductor, which can enable the promotion of both plasmon-induced charge and energy transfer processes. Our study can give a design guideline for devising heteronanostructure-based solar energy conversion platforms with intended functions.

Poster Presentation : **MAT.P-298**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Dual Functional 3D Star-Shaped Organic Semiconductors Enables Efficient and Stable Perovskite Quantum Dot Solar Cells

Seyeong Lim, Sungryong Kim[1], Taiho Park[*]

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

The CsPbI3 perovskite quantum dots (PQDs) exhibit superior optical and electrical properties such as tunable bandgap, multiple exciton generation, and excellent defect tolerance. Recently, the power conversion efficiency (PCE) of CsPbI3 PQDs solar cells was significantly boosted to over 15%, showing great potential as a promising optoelectronic material. However, during the layer-by-layer (LBL) deposit process, the use of polar solvents causes severe surface defects due to the ionic nature of the perovskite crystal structure. The moisture can penetrate into the PQD from the surface defect sites, further damaging the PQDs. Herein, we suggest a facile strategy which combines organic conjugated molecules with PQDs (i.e. Hybrid PQDs, HPQDs) to address the instability of PQDs. We newly designed a 3D star-shaped semiconductor material (Star-TrCl) with an excellent geometric balance of coplanarity and distortion characteristics. Their twisted 3D structure inhibits self-aggregation, increasing the compatibility of organic semiconductors with PQDs. The Star-PQD hybrid film significantly enhanced the phase stability by passivating the surface defect and preventing moisture penetration from hygroscopic HTM (Spiro-OMeTAD). Consequently, PCE was maintained at 72% even after 1000 hours in HPQDs device. Furthermore, the Star-TrCl constructed a cascade energy band structure, boosting PCE up to 16.0 %. So far, this is the most stable and efficient CsPbI3-based HPQDs. This 3D interface organic semiconductor design will provide a potential approach for commercializing the PQD photovoltaics.

Poster Presentation : **MAT.P-299**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fluorescent Liposomal Nanoparticles as a New Bio-imaging Agent Including Oxidized [5]CPP Aggregates

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Cycloparaphenylene (CPPs) are hoop-shaped molecules in which 5 to 12 or more units of benzene rings are para-conjugation. CPPs have significant attention due to their unique topology and unexplored properties in the bio-imaging research fields. However, the small size [n]CPP ($n < 7$) has non-fluorescence due to its optical selection rules. In addition, the small-size CPP has common problems with low water solubility, cytotoxicity, and low photostability. Recently, we confirmed for the first time the interesting physicochemical properties of oxidized [5]CPP (named Oxi-[5]CPP). In this study, we report on an easy strategy to produce a novel biocompatibility probe using Oxi-[5]CPP, which represents blue fluorescence. We constructed a novel bio-imaging probe by forming liposome nanoparticles (named Lip-[5]CPP) with Oxi-[5]CPP. And we systematically analyzed various liposome compositions through physicochemical analysis and established the most efficient and stable formulation. We confirmed the bio-imaging capability of Lip-[5]CPP by observing cellular uptake imaging using confocal laser scanning microscopy, and also demonstrated the potentiality of a two-photon imaging probe by two-photon emission properties analysis. We believe that our findings can affect not only basic research but also studies related to the formulation of the fluorescent probe.

Poster Presentation : **MAT.P-300**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Si-S bond formation on the porous silicon surface via microwave

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Porous silicon (pSi) materials have attracted attention in various biomedical fields for their benefits, such as superior biocompatibility, high substrate-loading efficiency, and facile surface modification. Therefore, it is important to study effective surface-functionalization for diverse applications of pSi. In particular, the hydrosilylation reaction with a pSi surface using the energy of heat, microwave, and light is most used widely. However, there is a limitation that this reaction must proceed under inert gas conditions to maintain an unoxidized surface such as Si–H on the surface of pSi.In this study, we disclosed a new and efficient surface-modification method, that can straightforwardly form Si-S bonds on the surface of pSi within 10 minutes, using the microwave. The microwave energy induced ring-opening reaction in the 1,2-dithiolane, which was a 5-membered cyclic disulfide compound, and formed the Si-S bonds more efficiently on the surface of pSi wafer than other methods (heating stirrer, ultrasonication, and vortexing). The reaction induced by microwave can also be applied to the pSi nanoparticles (pSiNPs), and the reacted pSiNPs showed low cytotoxicity. In addition, the reacted pSi maintained the original porous structure of pSi and a functional group (–COOH) that could be further functionalized derived from the 1,2-dithiolane. We believe that a new surface modification method with 1,2-dithiolane on the pSi surface through microwave can contribute to various fields by providing an efficient technique.

Poster Presentation : **MAT.P-301**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fluorogenic Materials for On-site Detection of Fire Blight Bacteria

Ji Hye Jin, Dokyoung Kim*

Department of Biomedical Science, Kyung Hee University, Korea

Fire blight is an infectious plant disease caused by *Erwinia amylovora* with symptoms that turns brown to black all over the plant organs. Because *E. amylovora* spreads rapidly and there is no cure for fire blight, it brings an enormous economic burden to agricultural industries, which increases yearly. However, conventional diagnostic techniques such as PCR, LAMP, and immunoassay-based strips have limitations with time-consuming, low field applicability, and extravagant specialized equipment. Accordingly, advanced fire blight diagnostic techniques have gained attention with on-site applicability and fast diagnostic time.In this work, we developed a novel diagnostic material, B-1, for fire blight based on fluorescence. B-1 is a turn-on type fluorophore that can selectively stain *E. amylovora* and exhibit near-infrared emission with emission peak of 686 nm. Compared with conventional diagnostic strategies, B-1 showed much higher sensitivity (limit of detection: 10^2 CFU/mL), and response rate (*E. amylovora* with concentration-dependent red fluorescence, gaining field applicability. We believe in the potential of B-1 as a most simple and powerful diagnostic tool without the necessity for an expert.

Poster Presentation : **MAT.P-302**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Photodynamic Therapy Material based on Porous Silicon Nanoparticles Targeting Glioblastoma

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Photodynamic therapy (PDT) is a minimally invasive therapy that uses specific light-sensitizing agents called photosensitizers. These agents induce the apoptosis of cancer cells by absorbing light of a specific wavelength to generate ROS. Indocyanine green (ICG), an FDA-approved photosensitizer for PDT, is a water-soluble cyanine dye with low toxicity and near-infrared photosensitive properties. Despite having PDT-optimized properties, ICG easily combines with serum proteins to induce rapid excretion and reduce optical properties by forming aggregates in water-soluble environments such as body fluids. In addition, ICG is photo-decomposed through the oxidative decomposition of polymethine, indicating poor light stability. To overcome these shortages, for the first time, we designed a glioblastoma-targetable photosensitizer consisting of three main components: i) pSiNPs: porous silicon nanoparticles are used as nanocarriers for surface chemical approaches and have excellent biocompatibility; ii) ICG: the ICG is used as an agent for PDT; and iii) SIWV (Ser-Ile-Trp-Val; tetra-peptide): SIWV can penetrate the blood-brain barrier and has GBM homing ability through caveolin-dependent endocytosis mechanisms. As a result, significant ROS was generated by the ICG in GBM cells and xenograft mice under NIR laser (808 nm) irradiation. The generated ROS further induced ICG releasing and ROS generation by accelerating the decomposition of nanocarrier pSiNP. We strongly believed that the potential of this interesting development has enough competitiveness to be a PDT tool, compared with approved probes.

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Poster Presentation : **MAT.P-303**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and electrochemical characterization of α-MnO_2 cathode 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 amorphous α-MnO_2 using $KMnO_4$ solution and tea extract as a reducing agent, and used as cathode materials for AZIBs. Subsequently, crystalline α-MnO_2 was obtained after the calcination of amorphous α-MnO_2. The electrochemical properties of amorphous and crystalline α-MnO_2 have been investigated systematically in order to elucidate the impact of crystallinity on the electrochemical intercalation/deintercalation of Zn^{2+}.

Poster Presentation : **MAT.P-304**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facet-selective Metal Deposition on 2D-Pt for Accelerated Hydrogen Evolution Reaction

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Herein, we introduce facile synthesis of 2D Pt-Metal nanohybrids having facet-selective interface (Metal: Pd, Ni). In this work, we utilized silica nanoreactor having aminated surface for well controlled metal growth reaction by concentrated metal precursor inside of nanoreactor. By utilizing it, we could synthesize porous 2D platinum nano-dendrites and 2D Pt-metal nanohybrids. Those secondary metal is deposited on 2D Pt's branch epitaxially with atomically thin layer (< ~1 nm). Based on our study, Pd and Ni has same FCC crystal structure and smaller lattice parameter than Pt. Thanks to these features, it seems that those metal-hybrid having well matched interface could be synthesized easily. Compared to that unique epitaxial growth, when we tried to grow secondary metal after removal of silica shell from 2D-Pt surface, Secondary metal filled 2D-Pt's pore to reduce porosity and surface free energy.Finally, as we introduce each Pd and Ni on 2D-Pt's different facet, we could synthesize Pt/Pd/Ni ternary-metal nanohybrid which is the most optimized catalytic platform for alkaline HER thanks to effective Pt-M interface having ultra-low overpotential and high mass activity compared to commercial 20 % Pt/C (η10 = 24 mV and 8 times improvement in mass activity). In conclusion, we could synthesize 2D Pt-metal nanohybrids by silica nanoreactor showing dramatic improvement in electrocatalytic HER. we are expecting that this facile strategy will give direction for facilitating diverse metal nanohybrids and synergistic effect applied in diverse field.

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Poster Presentation : **MAT.P-305**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Role of cations in 13X zeolites on the selective 1-octene adsorption

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1-octene, one of the linear alpha olefins, is used as a starting material in the petrochemical industry, such as surfactants and plasticizers. However, the major obstacle to obtain high-purity 1-octene is the separation and purification of 1-octene from 1-octene/*n*-octane mixture. In this study, the adsorptive separation of 1-octene from 1-octene/*n*-octane mixture have been investigated using ion-exchanged 13X zeolite adsorbents with different cations (Na^+, Li^+ Ca^{2+}, and K^+). Batch adsorption experiments have been conducted to determine adsorption properties for ion-exchanged 13X zeolite adsorbent. The adsorption capacity and separation factor of 1-octene for ion-exchanged 13X zeolites has been studied systematically as a function of cations and 1-octene fractions. In addition, the Langmuir constant (K_L)and heat of adsorption (ΔH_{ads}) were obtained through the Langmuir isotherm fitting and compared to elucidate the role of cations for the selective 1-octene adsorption.

Poster Presentation : **MAT.P-306**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Porous Aromatic Framework 41 Containing Nitrogen Element as Sulfur Support for High Performance Lithium Sulfur Batteries

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In recent years, lithium-sulfur (Li-S) battery has attracted tremendous attention due to the low cost, environmental benignity, high energy density. Despite of the high energy density, the intrinsic features of poor conductivity, high capacity decay, self-discharge inhibit the application of Li-S battery. A key problem is the shuttle effect that induced by the dissolved lithium polysulfides. Hunting suitable sulfur support is presently well-known an effect route to mitigate shuttle effect. Porous organic frameworks (POFs) feature in designable structure and composition, large surface area, tunable pore size, high thermal and chemical stability, and ready functionality. These characteristics render POFs promising sulfur support in Li-S battery. Here, N-containing porous aromatic framework of PAF-41 is synthesized and directly used as the sulfur support without any post treatment. PAF-41/sulfur composites (SPAF-41) were prepared by melt-diffusion strategy. The SPAF-41 electrode with high sulfur loading of 72 wt.% delivers a specific capacity of 725.8 mAh g^{-1} at 0.5 C at the first cycle. The sustained capacity of 491.4 mAh g^{-1} after 500 charge-discharge cycles at 0.5 C indicates an improved long-term cycling stability with a low decay rate of 0.06% per cycle.

Poster Presentation : **MAT.P-307**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Applications of high viscosity liquid gallium

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

Liquid gallium spontaneously forms a nanometer-thick thin oxide layer when exposed to air. By high-speed stirring, large amounts of this oxide skin can be generated and incorporated into the gallium bulk, forming stable and high-viscosity liquid gallium/oxide colloid. Here, we demonstrate some uses of this phenomenon, including its use as a heat transfer medium and as an alternative approach to foamed alloys of gallium. Particles that are typically immiscible with liquid gallium can be incorporated by using this method.

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Poster Presentation : **MAT.P-308**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Regulating Li-ion Migration at the Interface by Hybrid Carbon–$Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ Coating for Super-Fast Charge $LiFePO_4$ Cathode Material

Dung Nguyen, Jimin Kim[1], Youngil Lee[1,*]

Chemical Industry Research Institute, Core Research Institute, University of Ulsan, Vietnam
[1] *Department of Chemistry, University of Ulsan, Korea*

Lithium-ion batteries (LIBs) have become the primary power source for electric vehicles (EVs). Increasing energy density and fast charging capability with higher energy utilization have been considered critical for EVs 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 in the reverse direction during charge and discharge. In this study, we have found that $LiFePO_4$ (LFP) material coated with 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 (LFP@C_LATP) can be charged extremely fast. The solid-state reaction has been used to synthesize the LFP material and subsequent coating. Under the constant current charge-discharge protocol, the LFP@C_LATP can provide a charge and discharge capacity of 137.5 and 135.4 mAh g^{-1} at 10.0 C, which equals ~80% of the LFP theoretical capacity (170.0 mAh g^{-1}) and of about 1.3 times higher than the charge (108.1 mAh g^{-1}) and discharge capacity (106.9 mAh g^{-1}) of the conventional carbon-coated LFP (LFP@C) prepared at the same conditions. An adapted protocol containing multi-step constant current and then constant voltage charge can stably provide an average charge capacity of 161.7 mAh g^{-1} within 10 min, followed by a discharge capacity of 138.2 mAh g^{-1} at 1.0 C for 100 cycles.

Poster Presentation : **MAT.P-309**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Controlling supramolecular helicity of conjugated molecules by variation of the chiral alkyl spacer length

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Chirality is a common characteristic of nature, such as the right-handed β-form double helix of DNA, amino acids, and proteins. Chirality plays an important role in hierarchical architectures starting from the molecular to the supramolecular level. However, the mechanism of the formation of hierarchical structures from molecular to supramolecular level in the chiral self-assembly process is still far from being fully understood because chiral supramolecular structures are associated with a variety of factors such as noncovalent interactions (hydrogen-bonding, hydrophobic or hydrophilic interactions, van der Waals interactions, and π-π interactions) between molecules and external effects (temperature, solvent, pH, and additives). Therefore, investigating the chiral assembly according to molecular interaction will provide guidance on the design of new functional chiral materials. In this work, conjugated molecules with different chiral chain spacers were designed and synthesized. We control the chirality of supramolecular nanostructures through variation of the alkyl spacer length between the chiral chain and π-conjugated molecule. We discuss an investigation into how alkyl spacer between conjugated core and chiral side chains influence the internal arrangement of the π-π stacking within self-assembled molecules. Their electronic properties and morphology of the film were analyzed and characterized through various measurements such as UV–vis, photoluminescence, circular dichroism spectroscopies, and AFM.

Poster Presentation : **MAT.P-310**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Unusual Design Strategy of Quinoidal Conjugated Molecules for Supramolecular Chirality

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A number of chiral functional materials and their assemblies have been developed for decades due to their distinctively asymmetric structures and chiroptical properties for versatile applications including electronic/photonic devices, catalysts and medicines. In this work, we designed and synthesized novel quinoidal conjugated molecules QuEDOT-(S)-Cn and QuPheDOT-(S)-Cn employing enantiopure alkyl side chains. Due to the strong π-π stacking derived from highly planar structure of quinoidal molecules, their property was suitable for constructing supramolecular chirality. We will explain and discuss the behavior of supramolecular chirality in solution and film states depending on the types of solvents as well as different chemical structures. This result suggests the practical direction for inducing the supramolecular chirality of organic semiconducting materials.

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Poster Presentation : **MAT.P-311**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

$Cs_3(Cu_{2-x}Ag_x)I_5$ Crystals for Color Tunable Emissions

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We successfully synthesized the intrinsic $Cs_3Cu_2I_5$, and silver substituted $Cs_3(Cu_{2-x}Ag_x)I_5$ ($0 \leq x \leq 1$) perovskite in solution at room temperature to tune the emission color. We could control Ag content to obtain $Cs_3(Cu_{1.0}Ag_{1.0})I_5$ with Ag substitution of 50 % without side products such as $Cs_3Cu_2I_5$, Cs_2AgI_3. Depending on Ag content, the unit cell volumes and optical properties varied systematically. The crystal structure of Ag substituted $Cs_3(Cu_{2-x}Ag_x)I_5$ perovskite demonstrate incorporation of Ag^+ into the $Cs_3Cu_2I_5$ perovskite, indicating that all the X-ray diffraction peaks shifted monotonously to smaller angles with the increase of Ag^+ ions concentration. Also, $Cs_3(Cu_{2-x}Ag_x)I_5$ perovskites are still observed strong photoluminescence (PL) emission even after Ag substitution. The intrinsic $Cs_3Cu_2I_5$ polycrystalline Ag substituted $Cs_3(Cu_{1.0}Ag_{1.0})I_5$ polycrystalline shows an emission peaking at 445 nm, and 450 nm, respectively, associated with the self-trapped exciton emission.

Poster Presentation : **MAT.P-312**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Crystal structure and electrical property of complex perovskite oxynitrides $\mathbf{SrAl_{0.2}}\,\boldsymbol{M}_{\mathbf{0.8}}\mathbf{O_{2.4}N_{0.6}}$ (*M* = Nb, Ta)

Yang Hun Kim, **Young-il Kim**[*]

Department of Chemistry, Yeungnam University, Korea

Complex perovskites $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ (*M* = Nb, Ta) were synthesized by reacting Al_2O_3 with a layered oxide $Sr_5M_4O_{15}$ in an NH_3 atmosphere through a process consisting of the solid-state diffusion of Al^{3+} coupled with O^{-2}/N^{-3} substitution. Rietveld refinement showed that both $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ have a body-centered tetragonal symmetry ($I4/mcm$), and that the Nb phase, a = 5.7187(6) Å, c = 8.062(2) Å, V = 263.67(6) Å^3, has a larger volume than the Ta one, a = 5.7177(6) Å, c = 8.056(2) Å, V = 263.38(3) Å^3. In both phases, nitrogen favored the axial site over the equatorial site. Solid-state ^{27}Al magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy confirmed the six-coordinate environment of Al in $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$, hence verifying the phase purity of the samples. It is well expected that the mixed occupancies on the octahedral site and the anion site should cause significant local distortions in $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$. Indeed, the dielectric constant of $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ was measured to be as high as ≒600.

Poster Presentation : **MAT.P-313**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Au@Pt Nanohexapods through Isotropic Etching of Au with Pt Masks

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In this research, we designed a stepwise synthetic method for Au@Pt nanohexapods wherein the Au nanocrystals with a Cartesian-coordinate-like hexapod shape are tip-selectively decorated with Pt square nanoplates. Starting from Au nanocubes as a template, Au@Pt nanohexapods were successfully synthesized by applying three distinctive chemical reactions in a stepwise manner. The presence of Pt adatoms on the six concave facets of Au nanocrystal was the key element for generating hexapod morphology. These Pt adatoms formed discontinuous thin nanoplates that selectively covered specific facets and played a role as an etching mask which prevented underlying Au atoms from being oxidized. The subsequent isotropic etching proceeded radially starting from the bare Au surface without Pt mask, digging into the nanocrystal toward its center. The etching was timely stopped to avoid over-etching, so that the surviving Au domain consisting of core body and protruding arms could hold and link the Pt nanoplates, leading to the formation of Au@Pt nanohexapods. Due to their unique morphology, Au@Pt nanohexapods feature distinctive optical property of absorption in near-infrared region. We further extended our synthetic library by tailoring the size of Pt nanoplates, resulting in the Au@Pt nanohexapods having different size of Pt nanoplates on which a wide variety of catalytic reactions can take place.

Poster Presentation : **MAT.P-314**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Targeted combination therapy using paclitaxel encapsulated gold nanorod scaffolds

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The combination of different cancer treatment modalities such as chemotherapy (CHT) and photothermal therapy (PTT) synergistically improves the localization and therapeutic efficiency of anticancer drugs. Such multimodal approaches, simultaneously offer, localized heat-assisted killing and anticancer drug delivery, while reducing the unintended systemic side effects from a single therapy. However, the non-targeted effects of CHT-PTT lower their potency for direct cancer treatment. In this regard, considering the above limitations of CHT-PTT, we developed GNRs-based nanoplatform that improved drug accumulation via FR-targeted endocytosis. Briefly; GNRs were conjugated to pre-synthesized amphiphilic PPEG-Folic acid (PPFA) following electrostatic interaction. The synthesized PPFAGNRs considerably improved the loading and retained activity of paclitaxel (PTX).Whereas, the FA moiety in PPFAPTXGNRs promotes the accumulation of nanoplatform toward overexpressed FR.The increase in temperature caused by the GNR's plasmonic property upon near-infrared (NIR), irradiation (NIR) increased the release of PTX and gradually decreases the viability of cancer cells. In conclusion, our study clarifies that nanoplatform based on GNRs have the ability to transport hydrophobic drugs like PTX to target site and to have excellent synergistic effects when combined with CHT-PTT.

Poster Presentation : **MAT.P-315**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Hollow Structures of Reduced Graphene Oxide and LDH-derived Nickel Ferrite ($NiFe_2O_4$) as Anode Materials for Advanced Lithium-ion Batteries

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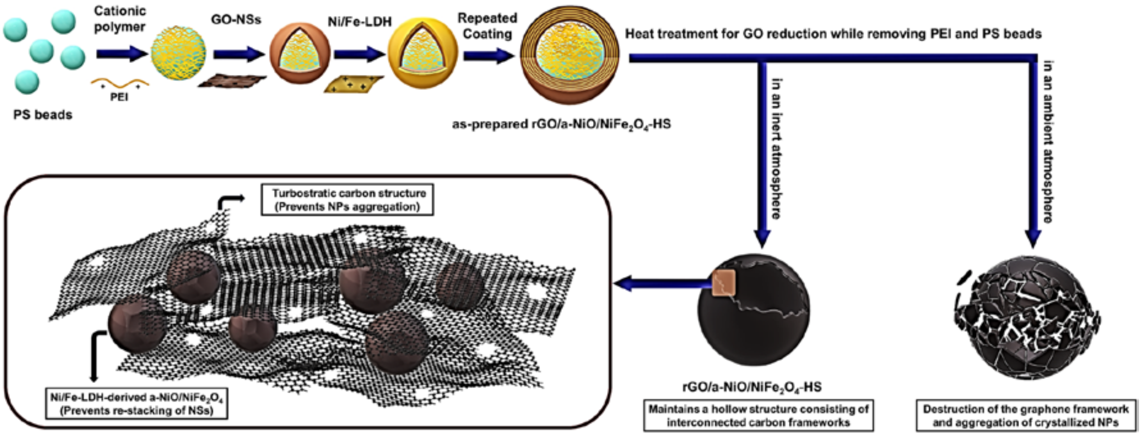
The increasing demand for energy storage devices and the expansion of the battery industry requires developing next-generation batteries with high energy density and stability. Among bimetallic compounds with more than twice the theoretical capacity of conventional graphite anodes, $NiFe_2O_4$-based anode materials have been attracted for their advantages, such as high energy density, natural abundance, and environmental friendliness. In addition, compared to pure metal oxides, hybrid strategies with carbonaceous materials have been reported to exhibit improved cycling performance due to the synergistic effects of the components. However, nanostructure control and homogeneous distribution of metal oxides in these hybrids remain challenging. In this study, we propose a novel carbonaceous hybrid design strategy containing $NiFe_2O_4$ derived from Ni/Fe-LDH. The rGO/a-NiO/$NiFe_2O_4$-HS, engineered with graphene nanosheets and Ni/Fe-LDH in a hierarchical hollow structure, provides an advantageous pathway for ion diffusion and effectively accommodates the volume change of metal oxide during the lithiation process. As a result, rGO/a-NiO/ $NiFe_2O_4$-HS provides a remarkable specific capacity of 1640 mAh/g at 100 mA/g after 550th cycles. Therefore, this hybrid system exhibits electrochemical synergy with the carbon matrix and metal oxides, providing new insights into nanostructured electrode design strategies.


Cationic polymer
PEI
PS beads
GO-NSs
Ni/Fe-LDH
Repeated Coating
as-prepared rGO/a-NiO/NiFe$_2$O$_4$-HS
Heat treatment for GO reduction while removing PEI and PS beads
in an inert atmosphere
in an ambient atmosphere
Turbostratic carbon structure (Prevents NPs aggregation)
Ni/Fe-LDH-derived a-NiO/NiFe$_2$O$_4$ (Prevents re-stacking of NSs)
rGO/a-NiO/NiFe$_2$O$_4$-HS
Maintains a hollow structure consisting of interconnected carbon frameworks
Destruction of the graphene framework and aggregation of crystallized NPs

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Poster Presentation : **MAT.P-316**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Termite repelling effect of melamine and catechol-modified cellulose and chitosan composites

Sanha Park, Jinkwon Kim*, Seog Woo Rhee*

Department of Chemistry, Kongju National University, Korea

In this study, modified composite materials were synthesized by the reaction of natural polymers cellulose and chitosan with melamine and catechol. Functional groups in the composites were analyzed through FT-IR analysis, and thermal stability of the composites was evaluated through TGA/DSC thermal analysis. The chemical structure of the composite and the relative ratio of functional groups were analyzed by ^{1}H NMR analysis. Coating of a filter paper was carried out by immersing a filter paper in an aqueous solution (or dispersion) of composite material. Subterranean termites (*Reticulitermes speratus*) prevention experiments were carried out in choice and no-choice tests. The composite materials applied to filter paper showed effective termite repelling and insecticidal effects.

Poster Presentation : **MAT.P-317**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation and characterization of dry bottom ash modified with $CaCO_3$ polymorphs

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, composite materials were prepared by adding Ca^{2+} aqueous solution and CO_3^{2-} aqueous solution dropwise to dry bottom ash (dBA, a concrete recycling material) dispersed in water, and growing $CaCO_3$ crystals on the surface of dBA. The dBA surface was coated with [(3-triethoxysilyl)propyl]succinic anhydride (TESPSA) and then hydrolyzed to introduce a negative charge to the surface. The composition, concentration and injection rate of Ca^{2+} and CO_3^{2-} solutions, reaction temperature and reaction time were adjusted so that only one phase among the polymorphs of $CaCO_3$, calcite, aragonite, and vaterite, was formed on the dBA surface. The morphology of the resulting composites was analyzed by FE-SEM, the vibrational modes of carbonate ions were analyzed by FT-IR, and the phases of $CaCO_3$ polymorphs were analyzed by powder XRD. On the dBA surface, a $CaCO_3$ monolayer with a size of several micrometers was formed. The hybrid composite materials prepared in this study can be used to control the hardening rate of concrete.

Poster Presentation : **MAT.P-318**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrolyte-gate thin-film transistor based biosensor using stable metal oxide semiconductor IGO

Euichan Jeon, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Field effect transistors (FETs) are being used in various ways in the field of biosensors. In this study, a biosensor using a stable metal oxide semiconductor IGO-based electrolyte gate thin film transistor was fabricated. Indium oxide was mainly used in biosensors using thin film transistors based on metal oxide semiconductors. However, there was a problem in that the frequency of occurrence of defective rates was high due to the high variability of the characteristics. So, we conducted research based on the IGO semiconductor, which has less volatility and is stable. To fabricate these sensors, the electrodes were passivated using 1,10-decanedithiol, Vinyl-POSS, Octadecanethiol, and the channels were immobilized with the aptamer to detect the target molecule. The manufactured biosensor was able to successfully detect Tau of various concentrations. In addition, since the biosensor is manufactured through a solution process, there is an advantage in that the sensor can be manufactured in a simple and low-cost method.

Poster Presentation : **MAT.P-319**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nanoscale Patterning of Semiconductor Surfaces to Enhance the Sensitivity of Electrolyte-Gated Field-Effect Transistor Biosensors

Jong Yu Song, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Biosensors based on electrolyte-gated field-effect transistors (EGFETs) are considered the most suitable platform for point-of-care diagnostics (POCD) among various biosensing devices. However, Debye screening, a phenomenon in which electrical double layers (EDLs) partially screen potential changes on the surface, occurs due to using electrolytes as a gating material in this system. This results in a significant decrease in the sensitivity of EGFET biosensors. To solve this issue, we utilized nanoscale patterns on the semiconductor surface, which are used as a sensing layer. These patterns were transferred from the master to the target surface via nanoimprint lithography (NIL) using poly(dimethylsiloxane) (PDMS) as a stamp material. The nanoscale patterning increased the number of binding sites by increasing the sensing layer's surface-to-volume ratio (S/V) while reducing Debye screening by suppressing the formation of EDLs in structurally concave regions. This enhanced the sensitivity of the EGFET biosensor. We anticipate that these fast, simple, and cost-effective approaches can be widely applied to various biosensors to improve the performance of POCD devices used in real-life scenarios.

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Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Ultrasensitive Extended-Gate Field-Effect Transistor (EGFET) based pH Sensor Using the Surface Modification of Sensing Parts

Hana Kim, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Recently, pH sensors have been utilized in various fields, such as basic research support, chemical and biological process monitoring, food manufacturing and processing, and environmental condition monitoring. The ISFET (Ion-Sensitive Field-Effect Transistor) used as a conventional pH sensor is made with the sensing part in contact with the electrolyte solution, which has the disadvantage that the passivation of the transistor is essential and unstable. To overcome these limitations, this study fabricated EG-FET (Extended-Gate Field-Effect Transistor) for a high-sensitivity and stable pH sensor. The fabricated EG-FET does not require passivation as the transistor and sensing part are separated from each other, and it is stable because the electrolyte solution does not directly contact the FET with an Extended-Gate. Furthermore, chemical modification on the Extended-Gate surface was employed to enhance the sensitivity and stability of the devices for pH sensing. First, this TFT is operated at a low voltage using a high-k ZrOx as a gate dielectric, and the semiconductor uses indium Gallium oxide (IGO). Heavily n++ doped Si wafer was used as the Extended-Gate and connected to the TFT. The Extended-Gate surface was amino-silanized with (3-aminopropyl)-triethoxysilane (APTES) for enhancing the performance of pH sensing. Finally, The EG-FET pH sensor fabricated by chemically modifying the Extended-Gate surface showed high sensitivity in the range of pH 4 to 10.

Poster Presentation : **MAT.P-321**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Non-Fluorinated Superhydrophobic Protection for Thin-Film Transistors by Multifunctional NPs-based-Nanocomposite Film

Leeun Park, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Thin-film transistors have recently been widely applied in the display field, among which organic thin-film transistors (OFETs) are a next-generation organic electronic device that is resistant to impact and can implement a device on a paper-like thin and flexible substrate through an inexpensive solution process. However, One of the long-standing problems in the field of organic electronics is their instability in an open environment, especially their poor water resistance. These problems also appear in oxide semiconductors. Herein, we fabricated a thermally stable and mechanically robust superhydrophobic protective film using multifunctional nanoparticles. The superhydrophobic protective film with excellent water-repellent and self-cleaning properties was synthesized by adjusting two types of alkyl silane to an optimal ratio in Si nanoparticles. Multifunctional nanoparticles have low surface energy due to the long alkyl silane and form a micro-nano hierarchical structure, so it is possible to fabricate a superhydrophobic surface. These multifunctional nanoparticles were deposited on semiconductors using a simple spin coating method. The protective layer has excellent resistance to mechanical and thermal stress and water threats without damaging the semiconductor. In addition, due to the superhydrophobic protective layer, more stable electrical characteristics were exhibited even when exposed to various ranges of pH such as water, KOH, and HCl.

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Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A study on flame retardancy of clay mineral/natural silk fibroin composite materials for the traditional Hanji

Sehun Jung, Byeongho Park, 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 carbonate anions was used as a clay mineral pigment. Silk fibroin was extracted from cocoons and used as a natural organic binder and coating agent. The thermal decomposition behavior of the composites was monitored by thermal analysis (TGA/DSC). Combustion test was performed up to 750 ℃ using a microcalorimeter on 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 rate (HRR) and the change in oxygen consumption as a function of time.

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Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Recovery of useful resources from sludge concentrated in gypsum washing water produced in desulfurization facilities

In Soo Koo, Sangchul Shin[1], Jinman Kim[1,*], Seog Woo Rhee[*]

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[1]*Department of Green Smart Architectural Engineering, Kongju National University, Korea*

Sulfur dioxide (SO_2) generated from coal power plants is converted to $CaSO_4 \cdot 2H_2O$ through a desulfurization facility. Washing water generated in the process of washing $CaSO_4 \cdot 2H_2O$ is concentrated under low pressure, converted into sludge, and landfilled. The main constituent ions of this sludge are Ca^{2+}, Mg^{2+}, Na^{+}, SO_4^{2-}, and Cl^{-}. Therefore, in this work, a process for recovering useful resources in sludge was developed by using the difference in solubility of ionic compounds in water. All sulfate ions were converted into $CaSO_4 \cdot 2H_2O$ by $CaCl_2$ treatment and separated into solids, and all magnesium ions were converted into $Mg_5(CO_3)_4(OH_2) \cdot 4H_2O$ by Na_2CO_3 treatment and separated into solids. NaCl remaining in the filtrate was concentrated and recovered as a solid, and the condensed water was recycled. The process developed in this work may contribute to the zero-discharge system, the ultimate goal of coal power plants.

Poster Presentation : **MAT.P-324**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of nano Si/SiOx coated graphite as an anode material for Li-ion battery

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

The lithium-ion battery has been using graphite as an anode material for about 30 years. Graphite shows small volume change and high coulombic efficiency in battery. But, recently, the low theoretical capacity of lithium-ion battery using graphite becomes a main defect. One of the strategies to get over this is adding Si to graphite anode. In spite of a high theoretical capacity of 4200 mAh/g, Si alone can't replace the graphite because of its poor cycle property. To solve this problem, the graphite with small amount of the Si can be used to decrease the effect of volume change of Si. In this study, a composite of Si/SiO_x and graphite was synthesized. The ball-milled SiO_x which contains SiO_2 and nano Si was used as a Si source. Milled SiO_x was mixed with carbon precursor, sucrose, and graphite. After the carbonization at 900℃, the nano Si/SiO_x-graphite composite was obtained. Synthesized composite showed higher capacity than graphite, not affecting the initial coulombic efficiency of the graphite.

Poster Presentation : **MAT.P-325**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Mesoporous Mn-Co-Ce catalysts for Preferential Oxidation of CO in H_2-Rich Stream

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

The Mesoporous Mn-Co-Ce mixed oxide catalysts were investigated for CO preferential oxidation (CO PROX) reaction, which was synthesized via nano-replication method using a hard template of KIT-6. The catalysts were characterized by X-ray diffraction, N_2 adsorption–desorption, H_2-temperature programmed reduction, CO-temperature programmed desorption and X-ray photoelectron spectroscopy. All of the catalysts had uniform mesopores and high surface areas. The distinct catalytic properties of these well-characterized mesoporous materials were demonstrated for preferential CO oxidation. Among them, the MCC-2 system presented the best CO conversion at low temperatures and the best selectivity toward CO_2. The received mesoporous Mn-Co-Ce mixed oxide possessed excellent textural properties. The structural stability was mainly attributed to the strong and stable interactions between cobalt oxides and manganese oxides.

Poster Presentation : **MAT.P-326**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Interfacial reaction between Ce-MOFs derived carbon and $KMnO_4$ to synthesize CeO_2-MnO_2 catalysts

Lianghao Song

Chemistry, Sungkyunkwan University, China

CeO_2-based catalysts are widely studied in the catalysis fields. Developing one novel synthetic approach to increase the intimate contact between CeO_2 and secondary species is of particular importance for enhancing catalytic activities. Herein, we design an interfacial reaction between MOF-derived Carbon and $KMnO_4$ to synthesize CeO_2-MnO_2, where the Carbon is derived from the pyrolysis of Ce-MOFs under inert atmosphere. The MOF-derived Carbon is found to restrain the growth of CeO_2 crystallites at high calcination temperature, and more importantly, the intimate contact within CeO_2/C is conveyed to CeO_2/MnO_2 after interfacial reaction, which are responsible for high catalytic activity of CeO_2-MnO_2 towards CO oxidation.

Poster Presentation : **MAT.P-327**
Material Chemistry
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Strengthen air stability of argyrodite structure type by element substitution and its replacement analysis by XRD analysis

Hyungjin Lee, Jihun Roh[1], Seung-Tae Hong[2,*]

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Li-ion batteries are utilized at various places. But the annual demand of electric vehicles and the amount of required energy are dramatically increasing. Nevertheless, the safety issue of Li ion batteries has been raised frequently. To overcome those kinds of problems, it is necessary to develop the post lithium-ion batteries. The sulfide solid electrolyte is one of the candidates because of its high density and ionic conductivity, but it is vulnerable for humid air. To solve the problem, here in, we substituted both metal and anion in pristine argyrodite structure which is from Li_6PS_5Cl to $Li_6M_xP_{1-x}S_{5-y}A_yCl$. According to Hume-Rothery rules, metal can be substituted only 0.01 ratio because of its ionic radius difference between metal and phosphorus. In anion substitution case, each sample2 and sample3 showed the best result, but still sample1 showed the best air stability. Compared with other samples, only sample1 can measure the EIS after 36 hour exposure and that ionic conductivity is maintained 54% compared to pristine. Furthermore, when the sample1 directly contact with oxide base cathode materials which is uncoated bare NCM811, the cycle is much stable than pristine. To figure out the substitution mechanism, Rietveld refinement is used for structure analysis. In the argyrodite structure, there are total three sites of sulfur. Among them, only sulfur 2 site is substituted by anion. In conclusion, metal and anion substitution can increase the air stability with maintaining the moderate ionic conductivity. Also, when we increase the bond strength between metal and sulfur 2 site, the air stable solid electrolyte will be discovered in the future.

Poster Presentation : **MAT.P-328**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Bioprinting Technique for Fabricating functionally Graded Hydrogel Architectures: 3D Ear Cartilage Structure with Locally Modified Mechanical Strength

Dongyoon Jang, **Kwanwoo Shin***

Department of Chemistry, Sogang University, Korea

The tissues of the human body are composed of cells and supportive tissues with various physical and biochemical properties. In particular, cartilage is a three-dimensional avascular microarchitecture with various mechanical strengths as a representative supportive tissue constituting an organ. Recently, as the three-dimensional cartilage structure can be easily realized by bioprinting, it has been of interest in research to imitate a structure with a functional gradient similar to the cartilage of the actual native ear tissue. We developed a bioprinting technique using functionally graded materials (FGMs) to simulate locally modified mechanical properties in fabricating human ear cartilage tissue. First, we designed a microfluidic active mixing printhead for extrusion of “on the fly” property-modifiable bio-ink. To test mixing capacity, the CaCl2 gradient channel was printed into a bath filled with Ca-cross-linkable alginate; optical microscopy showed that the diffusion length for the alginate bath differed depending on the concentration of CaCl2 in the medium. Further, we studied elasticity-modifiable hydrogel ink containing GelMA, sodium alginate, and PEGDA. This presentation will demonstrate how the active mixing module with property-modifiable ink can be used to print complex ear cartilage structures with locally tuned mechanical properties.

Poster Presentation : **MAT.P-329**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tracking transport dynamics of hydrogen on graphene via in situ surface-enhanced Raman spectroscopy

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Exploring the atomic or molecular transport properties of two dimensional materials is vital to understand their inherent functions and, thus, to expedite their use in various applications. Herein, a surface-enhanced Raman spectroscopy (SERS)-based in situ analytical tool for the sensitive and rapid monitoring of hydrogen transport through graphene is reported. In this method, a reducing agent, which can provide hydrogen species, and a Raman dye self-assembled on a SERS platform are separated by a graphene membrane, and the reduction of the Raman dye by hydrogen species transferred through graphene is monitored with SERS. For validating the efficacy of our method, the catalytic reduction of surface-bound 4-nitrothiophenol by sodium borohydride was chosen in this study. The experimental results distinctly demonstrate that the high sensitivity and rapid detection ability of SERS can allow the effective analysis of the hydrogen transport properties of graphene.

Poster Presentation : **MAT.P-330**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Phase Transfromation of Calcium Carbonate by Silk Fibroin

Byeongho Park, Sehun Jung, Seog Woo Rhee*, Jinkwon Kim*

Department of Chemistry, Kongju National University, Korea

In this study, Silk fibrin (SF) and sodium dodecyl sulfate (SDS) were used to control two phases of calcium carbonate by changing the reaction conditions. In general, the metastable vaterite phase transforms to the thermodynamically stable calcite phase. However, it has been found in our study that the most stable calcite phase formed with only SDS surfactant molecules could be transformed to metastable vaterite phase by addition of SF. The resulting calcium carbonate crystals were identified using FT-IR and SEM. The phase distributions of calcite and vaterite phases were monitored using XRD and the chemical compositions of the synthesized organic-inorganic composites were determined by thermal analysis (TGA/DSC).

Poster Presentation : **MAT.P-331**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Scalable synthesis of multicolored excitation-dependent emissive FeSe quantum dots in the organic and aqueous phase

Hyojin Kang, Jaebeom Lee[1,*]

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

Colloidal quantum dots(QDs) with a typical diameter size of 2-10nm are one of the great discoveries in nanoscience. They have unique chemical and physical properties such as diverse emission colors and bandgaps depending on their size. These QDs have been successfully applied in various fields such as optics, electronics, and biology. Among these, FeSe QDs which are typical layered transition metal chalcogenide nanomaterials have been reported to have a multicolored excitation-dependent emission (MEDE) property, unlike conventional QDs. In this research, we show the scalable synthesis of an optimized protocol with diverse synthetic parameters in organic and aqueous phases. Scale-up synthesis was carried out where 1L- and 5L- reactors were used to synthesize QD up to 20g. The QDs with optimized synthesis exhibited intense light blue fluorescence on 365nm exposure, which also displays strong photoluminescence and relatively high quantum yield in an aqueous system. (c.a.20%) Furthermore, the synthesized QDs in the organic phase conducted phase transition and PEGylation as a post-treatment process.

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Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and characterization of two-dimensional FeSe nanomaterials

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

Transition metal chalcogenides have recently attracted a lot of interest as promising nanomaterial for their unique properties and wide range of applications. In particular, FeSe has sparked renewed attention as two- dimensional layered structure as high-performance superconducting and thermoelectric materials and a viable approach for next-generation electronic devices. In this study, we report our recent works on optical and optoelectronic properties of FeSe two-dimensional nanoplates synthesized via hydrothermal routes. The samples were analyzed by powder XRD, TEM, SEM, AFM and UV-Vis spectroscopy. Creating novel 2D nanocrystals and discovering their exotic properties can be an effective approach to understand the universal bridge between the ordinary superconducting and Mott physics states.

Poster Presentation : **MAT.P-333**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Self-assembled rGO/TiO_2 Hollow Nanostructures for Enhanced Electrical/Ionic Conductivity as Anode Materials for Lithium and Sodium-Ion Batteries

Ji-Ho Park, Seung-Min Paek[*]

Department of Chemistry, Kyungpook National University, Korea

Titanium dioxide (TiO_2) has been regarded as a promising alternative anode material due to its abundance in nature, environmental friendliness, and low costs. However, several drawbacks including the low electrical/ionic conductivity have limited their practical applications in rechargeable batteries. In this study, to enhance the electrical/ionic conductivity of TiO_2-based anode materials, we synthesized reduced graphene oxide/titanium dioxide hollow spheres (rGO/TiO_2-HS) which fabricated via layer-by-layer self-assembly of exfoliated titanate and graphene oxide(GO) nanosheets with heat-treatment at 470℃ for 2h under argon gas flow. A single layer of GO, the highly conductive material, provides structural stability and fast charge transfer by sp^2-hybridized carbon atoms. These properties lead to enhanced electrical conductivity and rate capability. Meanwhile, the large surface area of hollow spheres facilitates the ion diffusion and access of electrolytes. As a result, the mixed phases of rGO/TiO_2-HS (layered TiO_2, anatase TiO_2, and bronze TiO_2) increased pseudocapacitance behavior during the storage process. Galvanostatic charge/discharge cycling exhibited enhanced reversible capacity of rGO/TiO_2-HS compared to TiO_2-HS. In addition, ex situ X-ray absorption near edge structure (XANES) spectra of rGO/TiO_2-HS remain nearly unaltered, which exhibited the long-term cycling stability of its electrode.

Poster Presentation : **MAT.P-334**
Material Chemistry
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Preparation and Growth Mechanism of NiTe and $NiTe_2$ Nanorods *via* a hydrazine reduction route

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[1]Department of Chemistry, Dongguk University, Korea

Nickel telluride is an important class of nickel chalcogenide that has recently gained extensive attention of various applications in the future aspects. Herein, we synthesized NiTe and $NiTe_2$ nanorods (NRs) *via* hydrothermal method using hydrazine reductant. To understand their growth mechanism, reaction held under similar conditions with just altering the tellurium content. It is found that when the ratio of Ni/Te is 1:1 and 1:2, products are articulate with hexagonal (NiTe) and trigonal ($NiTe_2$) crystal structures. During the reaction multiple roles of hydrazine were unzipping in the results of distinct phase structure and morphological analysis. Moreover, the Kirkendall effect based nucleation and growth mechanisms of nanorod with two different concentration of Te^{2-} ion role were studied with various techniques. Especially, TEM images clearly showed distinct images of hollow NiTe and dense $NiTe_2$ nanorods formation explains the effect of tellurium concentration. Therefore, results indicate that the nanorod-shaped NiTe and $NiTe_2$ materials have a promising potential role in catalysts, electronics, optoelectronics and so on.

Poster Presentation : **MAT.P-335**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of PVC/MoO_3 nanocomposite for fire-retardant applications

Zaheer Ahmad, Hyun Jung[1,*]

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

Two dimensional layered materials such as graphene, layered silicates, MoS_2, WS_2 etc., are well-known nanofillers that can provide enhanced mechanical, thermal, barrier and flame retardant properties in a variety of polymer matrices. MoO_3 nanosheets are expected to become one kind of useful fillers for improving the properties of polymers. However, because of the phase separation, MoO_3 is poorly dispersed into host polymer and make synergetic effect, which gives a weak improvement of host polymer. To achieve high-performance of PVC/MoO_3 nanohybrid, homogeneous dispersion of MoO_3 nanosheets in the polymer host matrix and proper interfacial interactions between the nanosheets and the surrounding matrix, we exfoliated MoO_3 then modified the surface of the exfoliated MoO_3 by organofiller cetyltrimethylammonium bromide (CTAB). The prepared material was analyzed for various characteristics using XRD, SEM, and TG. The XRD measurement, it can be seen the peak shifted to the lower angle resulting that the CTAB was successfully intercalated into the interlayer space between the layers of MoO_3. The morphology of the PVC/MoO_3 nanohybrid was determined from the SEM analysis. The thermal behavior of the nanocomposite was studied in detail by TG measurements depending upon the different weight percent of modified MoO_3 added.

Poster Presentation : **MAT.P-336**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication of magnetic nickel nanoparticles/mesoporous graphene composite and its characterization

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Transition metal nanoparticles have been studied with great scientific interest in recent decades due to their diverse properties, including catalytic, magnetic, electronic, and biological characteristics. However, the catalytic activity of nanoparticles can be significantly reduced when they aggregate during the production process by decreasing their specific surface area. To address this problem, in situ growth of metal nanoparticles on carbon-based supports is a promising solution. Here we report the synthesis of nickel metal nanoparticles supported on mesoporous graphene (NiMG) using electrostatic interactions between nickel hydrate ions and exfoliated graphene oxide. The mesoporous structure was designed using the tri-block co-polymer P123 as a soft-template. The as-synthesized material was further heat treated for carbothermal reduction in an argon atmosphere to convert nickel species to nickel metals. The obtained sample was characterized by different techniques. The X-ray diffraction patterns showed the obtained NiMG contains nickel metal without significant changes in the host MG structure, and N_2 adsorption/desorption isotherms result displayed the mesoporous structure of NiMG maintained with high BET surface area. Furthermore, the NiMG can have strong magnetic interactions with an external magnet.

Poster Presentation : **MAT.P-337**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and characterization of layered manganese oxide/mesoporous graphene nanohybrids

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[1]Department of Chemistry, Dongguk University, Korea

Layered manganese oxide (δ-MnO_2) has received considerable attention because of its wide range of electric, magnetic, catalytic, and photocatalytic applications, and their advantages such as low price and environmental compatibility, high theoretical specific capacitance, and redox capability. This layered manganese oxide (δ-MnO_2) improves the functionality of mesoporous graphene through the nanohybridization process. The porous hybrid structure of mesoporous graphene and layered manganese oxide with tuneable porosity and electrical properties could be used in the energy storage field as well as the mesoporosity of graphene controlled by layered manganese oxide content. Herein, δ-MnO_2 nanosheets were obtained by intercalation and delamination reaction of the protonic manganese oxide with the tetrabutylammonium (TBA) cation. And δ-MnO_2 hybrid with mesoporous graphene (δ-MnO_2/MG) was achieved by the interaction between layered manganese oxide (δ-MnO_2) and mesoporous graphene(MG). The characteristics of δ-MnO_2/MG were investigated with various techniques. In the future, these δ-MnO_2 and mesoporous graphene hybrid investigation features will create a more interesting impact.

Poster Presentation : **MAT.P-338**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication and characterization of lepidocrocite-type layered titanate as carbon felt electrode-coating for vanadium redox flow battery

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Two-dimensional (2D) metal oxide materials are widely used as electrocatalysts due to their superior redox capability, large surface area, easily tunable structure, and physiochemical stability. Specifically, titanium dioxide-based 2D materials such as lepidocrocite-type layered titanate are ideal candidates for applications in energy materials, either as electrode coatings or in making electrode composites. Here, we have synthesized negatively charged exfoliated colloidal sheets of layered titanate ($Ti_{2-x/4}\square_{x/4}O_4$; $x = 0.67$, □: vacancy) as coating materials on carbon felt electrodes of all vanadium redox flow battery (VRFB). Firstly, the lepidocrocite-type $Cs_xTi_{2-x/4}\square_{x/4}O_4$; $x = 0.67$, □: vacancy) was prepared using a conventional method, followed by the proton exchange of the cesium ion. The resulting protonated multilayer form $H_xTi_{2-x/4}\square_{x/4}O_4$; $x = 0.67$, □: vacancy) was delaminated with a bulky organic base, tetrabutylammonium hydroxide, into single sheets in a stable colloidal suspension. Although carbon felt has high electrical conductivity, it lacks active sites on its surface, has poor wettability, and weak electrochemical reversibility that leads to low electrode performance. As coatings, the as-prepared 2D exfoliated titanate electrocatalyst is expected to bridge these limitations by improving the electrode's physiochemical and structural properties, including its wettability, increasing active sites for vanadium redox reactions, and overall reaction kinetics.

Poster Presentation : **MAT.P-339**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Exploring multi-functional roles of quaternary ammonium salt in deep eutectic solvent-water binary electrolyte for high-performance electrochemical capacitors

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In electrochemical energy storage technology, a wide potential window in an electrolyte is essential for optimized supercapacitor functioning. However, organic electrolytes and ionic liquids, while having a broad potential window, have their own issues like safety risks (of organic electrolytes) and cost obstacles (of ionic liquids). To counter these problems, a new type of electrolyte based on deep eutectic solvents (DESs) has been declared as a viable option. DESs have numerous advantages, such as a wide potential window, nonflammability, cost-effectiveness, and ease of production. On the other hand, they suffer from high viscosity and low ion conductivity due to the robust hydrogen bonding among their components. To address these negatives, a new electrolyte has been created, which is a blend of DES and water. In this investigation, tetrabutylammonium bromide (TBABr) and ethylene glycol (EG) were utilized as the components of the DES. The inclusion of 50 wt% water to the DES increased ion conductivity from 1.64 mS cm^{-1} to 12.71 mS cm^{-1}, and decreased viscosity from 93.87 cP to 5.78 cP. Notably, the DES-water binary electrolyte retained its wide potential window > 2.4 V. It was found that the tetrabutylammonium cations created a hydrophobic film at the anode, which hinders the water reaction, as well as serving as a bromide complexing agent which enables a stable bromide redox reaction. When tested, the multi-functional electrolyte showed remarkable results, with an energy density of ~40 Wh kg-1 at 1 Ag-1 and a retention capacity of more than 80% after 3,000 cycles.

Poster Presentation : **MAT.P-340**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Solving Intrinsic Limitations of Static Zinc Bromine Batteries by utilizing multi-functional additive in Deep Eutectic Solvents with Water Co-solvent

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The utilization of static aqueous zinc bromine batteries presents a promising approach to sustainable energy storage due to their high energy, safety, and affordability. However, several encumbrances, such as the bromine shuttle phenomenon, the formation of Zn dendrites, and the side reaction of water molecules, have impeded the practical utility of these batteries. In the past, tetrabutylammonium bromide (TBABr) acted as an effective complexing agent to prevent cross diffusion of Br3-. Despite this, the limited solubility of TBABr in aqueous zinc bromine electrolytes remained a significant challenge. To tackle this issue, we opted to use a deep eutectic solvent (DES) with 30 wt% water serving as a co-solvent. The strong interactions between the components of DES enabled successful dissolution of TBABr. Additionally, the TBA component settled on the surface of the Zn to form a hydrophobic layer, which suppressed the growth of dendrites and inhibited water-related side reactions. The incorporation of TBABr into the construction of the static ZBB has enabled it to effectively seize the soluble Br3- that is generated from the cathodic reaction, thus preventing the emergence of dendrite formations on the Zn anode. This has resulted in batteries with a long shelf life (with retention of 80% after 6000 cycles at 5 A/g) and an excellent specific capacity (400mAh/g) even under high charge rates (25 C). Our innovative electrolyte engineering, encompassing a complexing agent and water in the DES, provides a cost-efficient and effective approach to fabricate advanced static ZBBs for practical energy storage applications.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **MAT.P-341**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Photocatalytic Adsorption of Benzene over Fe-oxide Modified AC

Lee Jea won

Sungkyunkwan University, Korea

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **MAT.P-342**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Enhancing the Electrochemical Performance of Redox-Enhanced Electrochemical Capacitors by optimizing the Electrode/Electrolyte Interfacial Interaction

Young Hun Cho, Seung Joon Yoo*

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

Poster Presentation : **MAT.P-343**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nanoantibiotics: Therapy of Drug-Resistant Bacteria

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To date, the misuse and abuse of antibiotics have amplified the bacterial-resistance, resulting in high mortality. In this flow, nano antibiotics (nAb) are rising clinical material not only to combat the surfed drug-resistant bacteria but also to reduce the development period for a new antibiotic. The nAb is defined as an antibiotic agent encapsulated with nanoparticle more than one. In addictions, the core components of nAb consist of organic/inorganic molecules.Herein, we disclose a new nAb that consists of an organic-metal complex (SANA). The part of an organic molecule in nAb is sceptrin isolated from the marine sponge as one of the natural compounds. Otherwise, the inorganic part consists of gold nanoparticles (AuNPs), which mainly is encapsulated in the organic component. Interestingly, the encapsulated AuNPs spontaneously formed in the sceptrin solution without any stimulus such as a reducing agent or heat. Au ion might be reduced by the pyrrole group of sceptrin, inducing the formulation of both nanoparticle and aggregate. Based on this, we systemically analyzed the characterization and bioactivity of SANA. The SANA demonstrated the large size of the organic part (~ 3 μm) with well-fine size (150 nm) of the encapsulated AuNPs as we measured the absorbance, dynamic light scattering, and transmission electron microscopy (TEM). In the biological test, the SANA showed excellent properties of nAb to drug-resistant bacteria in mouse blood with low toxicity to blood/endothelial cells. The bioactivity effect of SANA was verified by measuring the MIC, DCF, DiSC3, RT-PCR, and TEM analysis. Thus, our pioneering study proposes a new inspiration for the discovery of next-generation nAb that could overcome drug-resistant bacteria.

Poster Presentation : **MAT.P-344**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The application of treated molybdenum silicide through uncomplicated thermal progress as anode for lithium-ion batteries

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

Considerable researches have been devoted to the study of lithium-ion batteries (LiBs) in the past decades due to their high theoretical capacity and other properties, which like high charge retention, high volumetric and gravimetric specific energy, to be a high-performance LiB option. Metal silicides have advantageous features compared to other silicon-based anode materials, which are maintaining nano-structure during electrochemical reaction because of their high stability. In this study, we treated metal silicides under various temperatures and atmospheres. We characterized all samples by XRD, N2 adsorption & desorption, scanning electron microscope and electrochemical tests. Among them, molybdenum silicide (MoSi2) shows a remarkable transition. There were substantial structural and chemical transition throughout the calcination in air. And these transitions provoked compelling electrochemical improvements in reversible capacity and cycle retention.

Poster Presentation : **MAT.P-345**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Increased emulsion stability with Pickering: through hybridization of layered double hydroxide and deoxycholic acid

Kyoung Hyoun Lee, Hyun Jung*, Jae-Min Oh[1,*]

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[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Pickering emulsion: Emulsions with solid particles at the interface have attracted interest in various industries such as pharmaceuticals, cosmetics, textiles and agrochemicals due to their ability to resist against coalescence. Deoxycholic acid (DCA) hybridized with layered double hydroxide (LDH) was prepared by co-precipitation method. In dynamic light scattering studies, DCA-LDH maintained a significant small size (12%) in T at the bottom part (height 0–5 mm), which indicated particle concentration was reduced due to coalescence or Ostwald ripening. The emulsifying ability can be enhanced by interaction with LDH. The dynamic interaction between DCA and LDH greatly inhibited the molecular aggregation of DCA. Thus, formulations containing DCA-LDH acquired stability against aggregation. Pickering emulsions made with DCA-LDH have increased emulsion stability

Poster Presentation : **MAT.P-346**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

DFT calculation of La doped NiFe-LDH catalyst for an improved OER performance

Sanghoon Kim, Minho Kim[*]

Department of Applied Chemistry, Kyung Hee University, Korea

The oxygen evolution reaction (OER) is an important reaction to study because it incurs a high overpotential resulting from four-electron transfer, which makes difficult to optimize the reaction. In this study, we conducted density functional theory (DFT) calculations on La-doped NiFe-LDH as an OER catalyst. The NiFe-LDH structure was chosen because it has a lower overpotential than other LDH structures. We compared the DFT energetics of NiFeLa-LDH and determined how the overpotential changes as the amount of La changes. Our results show that La can stabilize OER intermediates through an elevated Fe d-band center, thereby reducing overpotential. Furthermore, we calculated the formation energy of O vacancies and confirmed that doping La promotes oxygen vacancy formation and reduces a band gap. Increased O vacancies can provide more active sites, and a reduced band gap can increase electrical conductivity.

Poster Presentation : **MAT.P-347**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Exploring Isovalent and Aliovalent Substitution in Superionic Chloride Solid Electrolytes and their Implications for Solid-State Batteries

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[1]*Department of Advanced Components and Materials Engineering, Suncheon National University, Korea*

Halide superionic conductors have recently emerged as potential solid-state electrolyte (SSE) materials for all-solid-state batteries (ASSBs) due to their intrinsic properties, such as high Li^+ conductivity, mechanical deformability, and excellent chemical and electrochemical oxidation stabilities compared to sulfide or oxide SSEs. In this study, we investigated the structural evolution and Li^+ migration of isovalent and aliovalent substituted Li_3InCl_6 with Er^{3+} (89 pm) and Hf^{3+} (71 pm). By substituting isovalent cations with similar properties, such as ($Li_3In_{1-x}Er_xCl_6$ ($0 \leq X \leq 0.5$)), the crystal structure can be improved through the creation of defects and vacancies in the lattice. Furthermore, introducing Aliovalent substitution ($Li_{3-x}In_{1-x}Hf_xCl_6$ ($0 \leq X \leq 0.5$)) with different properties can further enhance ionic conductivity, stability, and chemical flexibility of halide-based solid-state electrolytes. As a result, these benefits can lead to better performance in solid-state batteries and other electrochemical devices.The Rietveld refinement of neutron diffraction identified a monoclinic crystal structure over the entire range of substitution. Through isovalent and aliovalent substitution the Li^+ conductivity of Li_3InCl_6 drastically increased from 1×10^{-3} S cm^{-1} to a maximum of 2.5×10^{-3} S cm^{-1} at 30◦C. In addition, the electrolyte's conductivity can be restored after exposure to water, which can be useful in applications where moisture or humidity may be a concern. Additionally, the halide SSE exhibits excellent electrode interface stability towards oxide cathode materials ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) without any interfacial treatment. This isovalent and aliovalent mixed coordination compounds study paves the way for the effective use of low-cost halide superionic conductors in the development of next-generation, safer ASSBs

Poster Presentation : **MAT.P-348**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Coordination-Driven Self-Assembly of Spherical and Linear DNA Structures for Synthesis of Advanced Nanoparticle Clusters.

Jeesu Moon, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

Nanoparticle clusters (NPCs) are of great interest in the field of nanotechnology owing to their distinctive properties compared to those of the individual nanoparticles. To date, there have been numerous efforts to develop diverse NPCs based on a variety of molecular interactions. Despite the recent emergence as a new pathway to synthesize functional nanomaterials, DNA condensation induced by metal ion (M^{n+})-coordination has rarely been investigated as a tool for the synthesis of NPCs. In this presentation, we demonstrate a noble method for the synthesis of NPCs embedded in DNA matrices based on M^{n+}-induced condensation of linear and spherical DNA using thirty different M^{n+}s. Two types of the M^{n+}s are selected as representatives for further thermodynamic and kinetic investigation of their effects on the structures of the NPCs. As a model system of clusterization, gold nanoparticles (AuNPs) are employed to elucidate the synthetic mechanism based on their advantageous properties such as intense localized surface plasmon resonance and a large atomic number of Au, ideal for optical and electron microscopic analysis. Furthermore, our approach has also been successful for the synthesis of other types of NPCs using the similar approach, proposing its effectiveness as a versatile strategy for the synthesis of NPCs.

Poster Presentation : **MAT.P-349**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tunable band edge positions of CQD films by fractional ligand replacement

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[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Colloidal quantum dots (CQDs) have captured significant attention as a promising next-generation material because of their exceptional electronic properties that can be modified via surface engineering. The surface modification technique of ligand-replacement allows the manipulation of the band edge position of CQDs through the reconstruction of the dipole layer on their surface. However, this method may not be compatible with the original fabrication process of CQD layers, which involves considering the solubility and wettability of CQD layers. This study addresses this challenge by utilizing a fractional ligand replacement process that enables the tuning of the band edge position while preserving the favorable properties of CQDs. Photoelectron yield spectroscopy was utilized to investigate the shift in band edge positions, which eliminates the charge-up problem that arises due to pristine long-insulating ligands. The findings demonstrate a linear relationship between shifts in the band edge positions of CQDs and the fractional ligand replacement process, providing a guide to optimize the band alignment of CQD layers for use in CQD optoelectronic devices.

Poster Presentation : **MAT.P-350**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Role of $ZnCl_2$ in synthesis of single-crystalline InP tetrapod nanocrystals

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Department of Energy Science, Sungkyunkwan University, Korea

Recently, Indium phosphide (InP) tetrapods were able to successfully synthesize as a single crystalline structure, which allowed for the examination of multiple exciton behaviors. To improve the optical performance, the researchers used $ZnCl_2$ precursor, a commonly used additive in the synthesis of aminophosphine-based InP nanocrystals. We synthesized InP tetrapods with addition of $ZnCl_2$ (InP-$ZnCl_2$) with a narrower arm length distribution. Interestingly, the addition of $ZnCl_2$ did not result in a distinct enhancement in photoluminescence and suppressed with arm length in the InP tetrapod. However, further shell growth on InP-$ZnCl_2$ successfully preserved the tetrapodal geometry in InP-$ZnCl_2$/ZnSe and showed higher photoluminescence than that of tetrapodal InP/ZnSe. Additionally, the crystal structure of InP-$ZnCl_2$ was maintained even with various Zn feed ratios as observed through x-ray diffraction (XRD) patterns, indicating that Zn only passivates the surface of InP tetrapods. These results offer a useful platform for studying the role of the Zn precursor.

Poster Presentation : **MAT.P-351**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Practical application of magnesium-based magnetic nanosheets for the removal of toxic organic pollutants

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[1]*Division of Chemistry and Bio-Environmental Sciences, Seoul Women's University, Korea*

Despite their high surface area and efficiency, nanoparticles are limited in their application in wastewater treatment due to potential toxicity, secondary pollution caused by their discharge into the environment, and recovery problem. Here, magnesium-based magnetic nanosheets (MMNs) which were easily prepared by a simple molten salt method were employed as an adsorbent for toxic organic dyes. Since MMNs are positively charged 2D materials, they were electrostatically deposited onto a sponge by layer-by-layer method with negatively-charged polyelectrolytes. Not only by a batch-type adsorption test using powder itself, but also an adsorption test using a sponge, MMN demonstrated excellent adsorption efficiencies for negatively charged organic contaminants. Due to the economical synthetic process and the variety of techniques applicable to the removal of organic pollutants, these MMNs show great potential in the field of wastewater treatment.

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **MAT.P-352**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Chiral Indium Phosphide Magic Sized Clusters: Structure and Chirality

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Magic Sized Clusters (MSCs) are small sized inorganic nanoparticles which are less 2 nm in size with a thermodynamically stable structure. Their highly surface-dependent properties, MSCs are found to have various types of isomers. Particularly, isomers which exhibit dissymmetric circular dichroism signals, also known as optical isomers, are discovered by the authors. We introduce chiral InP MSCs with unprecedented large circular dichroism signals compared to previously reported chiral semiconductor nanocrystals. To investigate the chiroptical origins of our chiral MSCs, characterizations including XRD and Raman were conducted to explore ligand geometry and structural properties. By surface characterizations including FT-IR and TGA, we have found that cysteine exists in the form of double anchoring modes. By structural characterizations, our MSCs were observed to exhibit polytwistane crystal structures. Chiral InP QDs with similar diameter were prepared with analogous methods, whereas the optical activity was silent. We speculate that low crystal symmetry and large transition dipole moments of MSC gives high chiroptical activity, whereas high crystal symmetry and low transition dipole moments of QD gives nearly silent chiral signal. Using chiral InP MSCs as templates, we could synthesize InP QDs, which in this case chiroptical activity was observed. Also, we could introduce halide atoms (Cl, Br, I) as dopants into chiral MSCs, which was also optically active. Our findings emphasize the unique characteristics of MSCs as prospective chiral materials and give intuition on designing chiroptical nanomaterials.

Poster Presentation : **MAT.P-353**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Manganese-based nanocatalysts for fast degradation of azo dyes

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[1]*Division of Chemistry and Bio-Environmental Sciences, Seoul Women's University, Korea*

Manganese oxide nanoparticles have attracted intention as effective catalysts for the degradation of azo dyes in wastewater treatment due to a high surface area, chemical stability, redox properties and cost-effective materials. Here, mono- and bimetallic manganese oxide nanoparticles (MON) were synthesized by a simple molten salt method in 1 min. Monometallic Methyl orange (MO), the most popular azo dye, were tested for catalytic degradation using MON nanoparticles, which demonstrated excellent degradation ability of 95% within 4 min under acid condition (pH=2). Various MON nanoparticles were employed for catalytic degradation of various azo compounds such as Orange II, methyl red, and Congo red, and the catalytic reaction mechanism was investigated by comparing the their catalytic efficiencies.

Poster Presentation : **MAT.P-354**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis and Mechanism Studies of Ag-Au-S alloyed Nanocrystals via Cation Exchange

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

Silver, gold, and their alloy chalcogenide nanocrystals (NCs) have narrow band gaps which range from red to short-wave infrared. They are free from heavy metal elements such as Cd, Hg, and Pb, which makes them ideal candidates as environmentally-friendly or non-toxic infrared probe material. Silver chalcogenide (mainly Ag2S and Ag2Se) NCs have been intensively studied for many potential applications that include infrared photodetectors and bioprobes. However, they suffer from low chemical and electrical stability which inherently originates from the low lattice energy and high mobility of Ag ions. Here, we report synthesis of Ag-Au-S alloyed NCs (Ag2-xAuxS) via cation exchange from Ag2S NC. The role of halide and phosphine in the cation exchange reaction has been studied. Reactions with halides are found crucial for the enhancement of cation exchange to reach the complete cation exchange forming precipitates, whereas the use of phosphines hinders such precipitate formation, limiting complete cation exchange. We report the photoluminescence (PL) properties of Ag2-xAuxS NCs for the first time. The chemical composition Ag2-xAuxS NCs were flexibly tailored to tune the PL emissions. The brightest Ag2-xAuxS NCs showed improved PL efficiencies of up to hundreds of times over Ag2S NCs. We hope that this novel strategy will expand ways to synthesize other materials as controlling the reaction steps and optical properties. It is also expected that these PL enhanced heavy metal-free NCs should be utilized in bioimaging, LEDs, and photovoltaic devices.

Poster Presentation : **MAT.P-355**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Highly porous cobalt ferrite magnetic nanospheres with ultrahigh removal efficiency for organic dyes

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Cobalt ferrite has attracted attention in the field of wastewater treatment due to its distinct magnetic, catalytic, and adsorption properties. Herein, magnetic cobalt ferrite oxide nanosphere, Co_2FeO_4 with high porosity (133.2 m2g-1) were prepared by a one-step solvothermal method. The Co_2FeO_4 nanospheres exhibited over 95% removal efficiency for anionic organic pollutants, methyl blue and Congo red with calculated maximum adsorption capacity of 1,400 mg/g and 940 mg/g at 313 K, respectively. In addition, Co_2FeO_4 completely decomposed a cationic pollutant, methylene blue (MyB) within 20 min in the presence of oxone. After the adsorption and catalytic reactions, the Co_2FeO_4 nanospheres could be easily isolated from the solution by external magnet. Due to an economical synthetic process and a variety of techniques applicable to the efficient removal of a wide range of toxic organic contaminants, the Co_2FeO_4 nanospheres show great potential in the field of organic wastewater treatment.

Poster Presentation : **MAT.P-356**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Useful Pendant Polymer for Effective Charge Carrier Transport through Regulating the Supramolecular Self-Assembly

Byeong hwak Bae, Jin Kuen Park[1,*]

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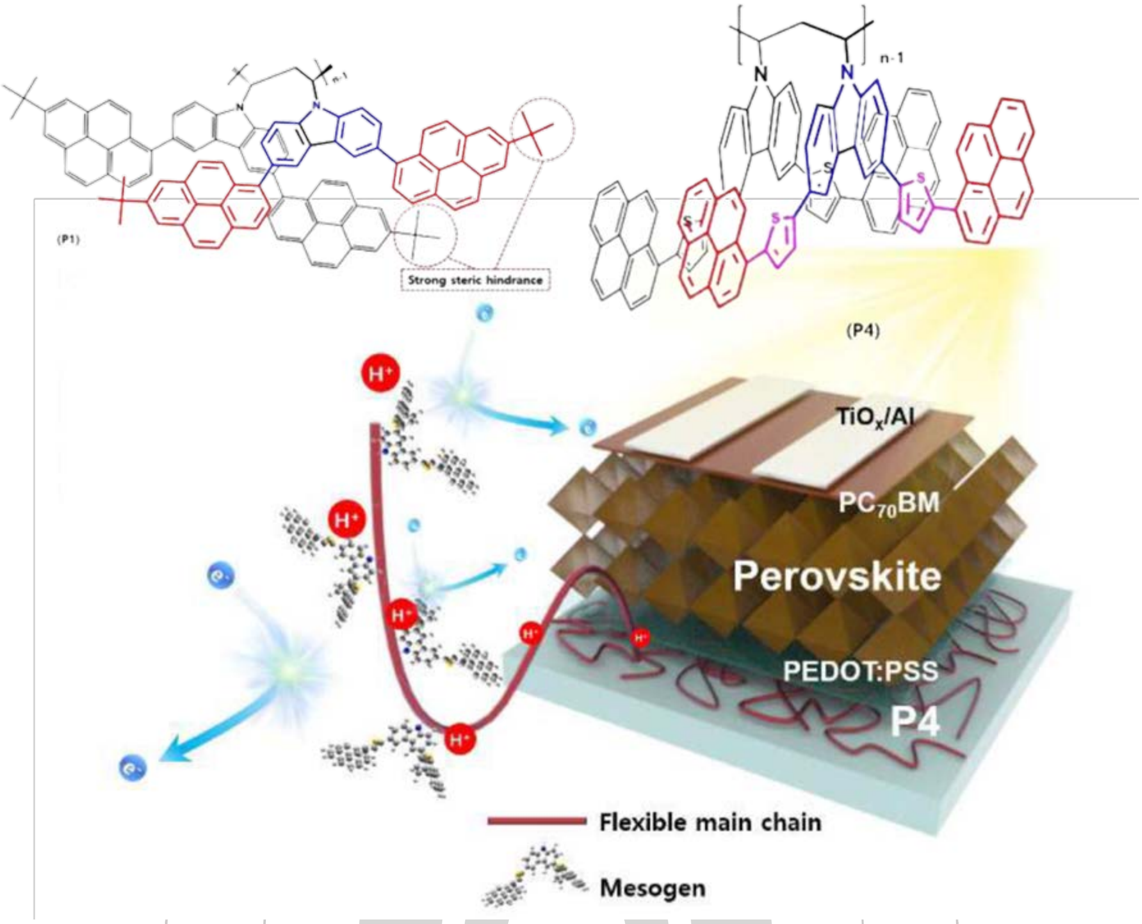
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Pendant polymers (polyvinyl carbazole, P0) were prepared by renovate carbazole motifs with pyrene used derivatives (P4 and P1) for enlarging the bandgap or highest occupied molecular orbital and lowest unoccupied molecular orbital energy levels. To define the electronical properties of pendant polymers which has carbazole motifs according to different structure, the polymers were applied to hole transport layer to perovskite solar cell (PSC) and organic photovoltaic cells (OPC). When thiophene-pyrene attached polymer (P4) was used for HTL, every device parameter without open-circuit voltage, was improved comparing with P0 and P1 (π-π conjugated by t-butyl pyrene motifs). Because P4 has higher electrically conductive properties of thiophene than benzene motifs of fewer alkyl chain, the supramolecular self-assembly structure of P4 indicated to be more available in electronic devices. Additionally, devices with P4 indicated to have smaller dark current than others which could be responsive to photo detecting devices and effective for charge carrier transport.


(P1)
n-1
N
Strong steric hindrance
(P4)
n-1
N
S
H+
TiOx/Al
PC70BM
Perovskite
PEDOT:PSS
P4
Flexible main chain
Mesogen

Poster Presentation : **MAT.P-357**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Two-Dimensional Array of Organic/Inorganic Hybrid Electrodes for Developed Electrical Conductivity toward Lasting and High-Performance of Sodium-Ion Batteries

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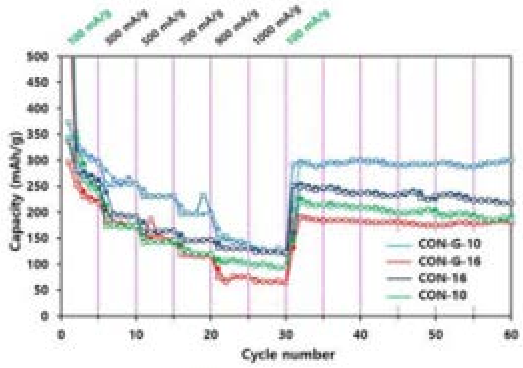
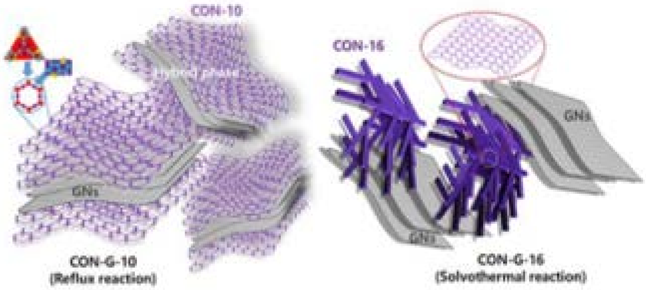
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

To research the influence of electrical conductivity upon the energy-storage features of sodium-ion battery anode materials, covalent organic nanosheets; they mean CONs, are synthesized to hybridize with graphene nanosheets (GNs) that have high conductivity via two different methods: solvothermal and reflux synthesis routes. The reflux-synthesized hybrid displays a well-overlapped 2D arrangement, whereas the solvothermal-synthesized hybrid fashions a segregated phase where the contact surface between the GNs and CONs is reduced. These hybrids synthesized by simplistic methods are completely identified, and the results tell improved energy-storage features by boosting the electrical conductivity by way of arrangement of a well-overlapped organization between CONs and GNs. The reflux-synthesized hybrids have higher discharge capacity and rate ability than the bare CONs, accentuating that the advances in charge carrier transport features can improve the approachability of Na+ to the connection area of the hybrids. This synthetic process can be improved to make advanced anodes for SIB systems.


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
CON-G-10
CON-G-16
CON-16
CON-10
0
10
20
30
40
50
60
Cycle number


CON-10
Hybrid phase
GNs
CON-G-10
(Reflux reaction)
CON-16
GNs
GNs
CON-G-16
(Solvothermal reaction)

Poster Presentation : **MAT.P-358**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Layered Cobalt and nickel hydroxide single layers as an efficient catalyst for the p-nitrophenol reduction reaction

Han kyeol Bae, Jong Hyeon Lee*

Department of Chemistry, The Catholic University of Korea, Korea

The nanosheet catalyst consisting of cobalt and nickel hydroxides was developed using a liquid exfoliation of bulk-layered metal hydroxides. These exfoliated cobalt/nickel hydroxides are a heterogeneous catalyst for reducing the p-nitrophenol under sodium borohydride. The alpha-Co(OH)2, known as hydrotalcite-like materials, has positively charged hydroxide layers with expanded interlayer spaces, charge-balancing anions, and water molecules. This study found that the exfoliated cobalt hydroxide showed excellent catalytic performance compared with its bulk cobalt hydroxide, cobalt chloride, and even commercial Pt/C. We assumed that the Co(II) cations in the hydroxide layer quickly turned into a CoBx under NaBH4 conditions, which effectively catalyzed the p-nitrophenol during the reduction reaction. A CoCl2, which also yields the Co2B complex, quickly aggregates into large particles during the catalysis, showing a low catalytic activity. Interestingly, our nanosheet catalyst exhibited excellent activity and stability compared to Co2B during the reduction of p-nitrophenol. Their high catalytic activity and stability are mainly ascribed to the well-dispersion in solution without significant aggregation compared to their bulk cobalt hydroxide and Co2B.

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Poster Presentation : **MAT.P-359**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

In_2TiO_{5-x} incorporated with $MoSe_2$ nanolayers for Photoreduction of CO_2 to CH_4 : A DFT Study

Myeongjin Jang, Minho Kim[*]

Department of Applied Chemistry, Kyung Hee University, Korea

Photocatalytic reduction of CO_2 into organic molecules such as methane would allow renewable energy sources. To enhance photocatalytic efficiency, considerable efforts have been devoted with diverse strategies. In this work, we studied the mechanism of CO_2 reduction on $In2_2TiO_{5-x}/MoSe_2$ catalyst model based on density functional theory (DFT) calculations. In a catalyst model, a Ti^{3+} state is obtained by a photoexcited electron and an oxygen vacancy. Ti^{3+} with a localized electron provides an active site of CO_2 reduction, while In^{3+} provides an adsorption site for H_2O. Hybridization with a $MoSe_2$ nanolayer can improve the photoreduction efficiency by modifying the electronic structure of In_2TiO_{5-x}. It allows charge transport to increase the electron density of In_2TiO_{5-x}, and CO_2 can receive more electrons. $MoSe_2$ nanolayer also appropriately modifies the energy band levels for the reduction of CO_2.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **MAT.P-360**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Formation of Wrinkling Patterns for Flexible Electrodes by Using Direct Printing

SeungYeon Lee, Kwanwoo Shin[1,*]

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

For flexible electronics, a flexible electrode is an essential element while maintaining conductivity under repeated bending and folding. A wrinkled electrode on elastomeric substrate has received much attention as an effective way to fabricate flexible electrode. However, fabrication of flexible electrode needs pre-stretching or thermal expansion of the substrate which is time-consuming and hard to fabricate customized circuit design. In this study, the wrinkled electrodes can be printed and formed by a simple direct printing. Triethylene glycol monoethyl ether (TGME) as a solvent of silver nanoparticle (AgNP) ink induced the permanent buckling on the top layer of elastomer. The condition of printing is optimized to fabricate stable electrode regarding to the size of needle, oxidation time, printing speed and ratio of PDMS. The wrinkling pattern helps to increase repeatability and stability of conductivity under mechanical bending compared to the non-wrinkle electrode. With this simple fabrication method, we produced an electrochemical sensor which has high sensitivity and durability under finger bending motion. This could be used in on-site detection of glucose, lactate, or other physiological parameters.

Poster Presentation : **MAT.P-361**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication of Controllable Hydrogel-Based Hollow Structure by using negative 3D printing for Future Artificial Organ

Yeeun Cho, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Fabrication of hollow organs such as the vascular system, digestive and respiratory tract, which comprise our body, received enormous concern in biomedical engineering development for transplantation. Current approaches for 3D bioprinting of hollow structures have achieved important advances but still require significant development. We develop a novel 3D bioprinting technique to directly fabricate and control complex hollow structures, mimicking the shape of the hollow organs. In this method, diffusion is the important key by incorporating calcium chloride in Pluronic F127 (PF127-Ca) as a fugitive ink and subsequently casting alginate and gelatin mixture over the extruded PF127-Ca. After extruding PF127-Ca on the top of the alginate-gelatin mixture, calcium ions will diffuse, crosslink the alginate, and yield a hollow hydrogel construct that physically mimics the hollow organs. This method allows for hierarchical bifurcation and complex hollow shape from macroscale to microscale, enables easy control over the wall thickness of hollow structure and the mechanical properties of fabricated hollow shape through additional process. Plus, with a simple change in 3D modeling, the inner microarchitectures of natural organs can be mimicked directly during the process. The fabricated hollow structure, mimicking the native organs, provides a potential platform to study artificial organs to transplant.

Poster Presentation : **MAT.P-362**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Core(Au)-Gap-Shell(Pt) Structure Dependent on Surfactant Halide for Enhanced Photocatalytic Activity in Low Laser Power

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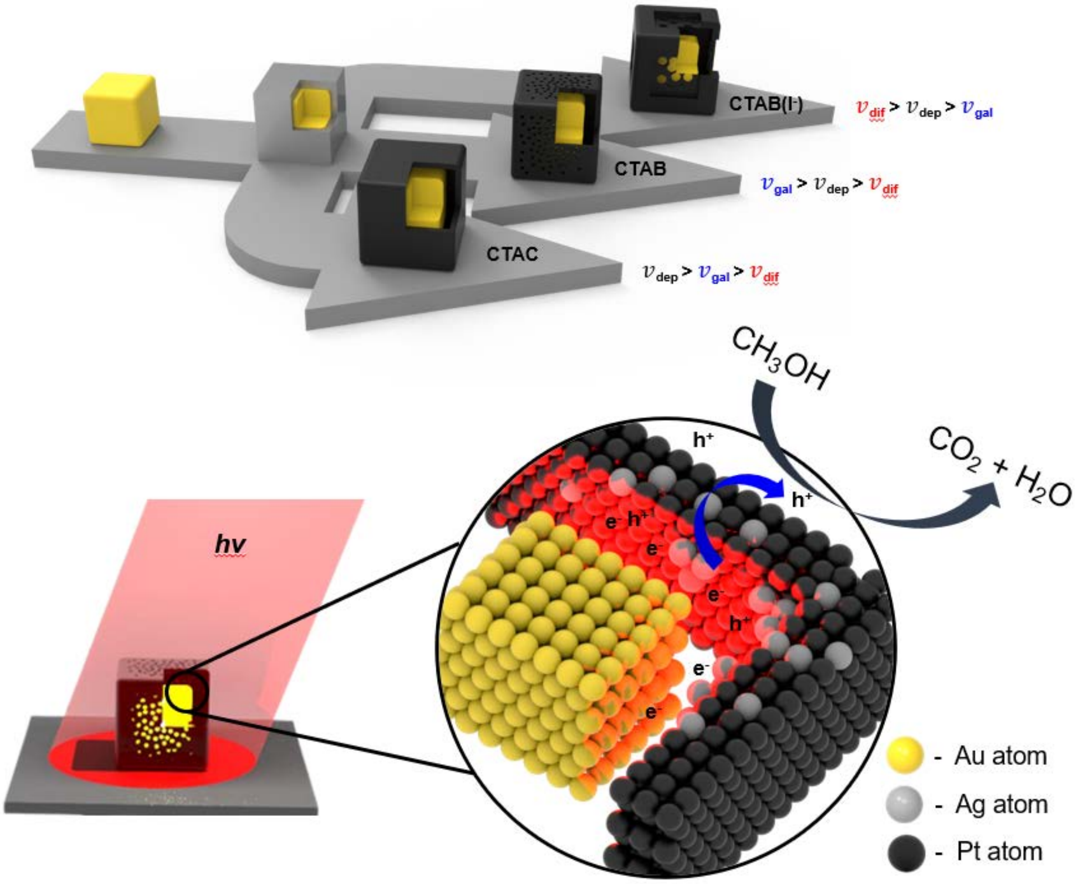
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Controlling surfactant of nanoparticles for changing morphology is widely used method for fabricating nanoparticles. Especially in the CTA^+ based cationic surfactant, anionic effect of halides(Cl^-, Br^- and I^-) shows considerable differences, and also it shows differences in galvanic replacement reaction between Pt and Ag or Au and Ag. Using this method, we successfully synthesized three kinds of Core(Au)-Gap-Shell(Pt) nanoparticle; cube in a shell, cube in a cage and cube in a frame from Au@Ag nanocubes. As changing surfactant anion, we could control not only morphology but also plasmonic effect in methanol oxidation reaction(MOR). In this MOR, plasmonic Au core absorbs light, so excited surface plasmon on the surface of inner core can generate hot carriers for catalytic reaction. Even MOR activity is radically increased in low laser power condition. Based on this result, Core(Au)-Gap-Shell(Pt) nanoparticle can be widely used for real world photocatalyst because of catalytic enhancement in low laser power condition.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CTAB
$v_{gal} > v_{dep} > v_{dif}$
CTAC
$v_{dep} > v_{gal} > v_{dif}$
hv
CH_3OH
$CO_2 + H_2O$
h^+
h^+
e^- h^+
e^-
e^-
h^+
e^-
e^-
- Au atom
- Ag atom
- Pt atom

Poster Presentation : **MAT.P-363**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Boron-doped cobalt hydroxide nanosheet for efficient oxygen electrocatalysis

Han Bi Kim, Jae Hyeon Nam[1], Jong Hyeon Lee[*]

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

A potential increase in global-energy demand has prompted extensive research on producing renewable energy and energy storage systems. Electrocatalytic water splitting using electric power is an effective method for producing chemical fuels with minimal environmental damage. However, the oxygen evolution reaction (OER) slows the water splitting because of its sluggish electron-transfer kinetics compared to the hydrogen evolution reaction. Noble-metal-based compounds, such as RuO_2 and IrO_2, are considered the most active OER catalysts; however, their natural scarcity and expensive nature hinder their practical use. In this study, we suggest a noble catalyst film consisting of a cobalt hydroxide nanosheet and its boron-doped derivate. First, the nanosheet of cobalt hydroxide was prepared using a liquid exfoliation of bulk alpha cobalt hydroxide, which has positively charged hydroxide layers with expanded interlayer spaces, charge-balancing anions, and water molecules. Then, a wet $NaBH_4$ treatment turns the $Co(OH)_2$ nanosheet into the boron-doped $Co(OH)_2$ nanosheet, exhibiting a high OER activity and stability under 1M KOH solution.

Poster Presentation : **MAT.P-364**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Deteriorating effect of transition-metal doping on Ni-based layered double hydroxide for glycerol oxidation at low potential

Min Seok Lee, Minho Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Increasing consumption of eco-friendly energy promotes research interest on alternative energy resources. Accordingly, one of biomass energy sources, study on glycerol electro-oxidation reaction (GEOR) is getting attention to utilize the excess glycerol in the biodiesel industry and save preprocessing costs so that the efficiency of biodiesel plants can be maximized. As GEOR proceeds, various by-products including formic acid (FA), which is a maximally oxidized form, are produced. For a GEOR catalyst, noble metals such as Au, Pt and Pd have been previously used, though they're expensive. In this study, DFT simulation of GEOR was conducted with Ni LDH, which contains an earth-abundant transition metal, for reducing costs and to see the efficiency by incorporation with Fe. As a result, the GEOR reaction using NiFe-LDH requires 0.12eV higher onset potential than with Ni LDH.

Poster Presentation : **MAT.P-365**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Precursor-Dependent Byproduct Formation and Structural Stability of Bimetallic Mesh Nanostructures Replicated on AgCl

Han-Jung Ryu, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

AgCl nanomaterials have recently attracted scientific interest as convenient structural building blocks for the synthesis of metallic nanomaterials owing to their facile synthesis, controllable morphology, and easy removal under ambient conditions. However, their complex chemical reactivity has often been studied mainly in association with water-solubility or reducibility. In this study, we investigate the pivotal role of precursor ligands in the photochemical synthesis of metallic cubic mesh nanostructures on the AgCl templates. The side reactions between AgCl and Au precursors with different ligands are thoroughly demonstrated, including their influence on the side reactions and structural stability of the resulting metallic nanostructures. Importantly, we unveil for the first time the partial destruction of AgCl and formation of undesirable byproducts caused by highly oxidizing and Cl-containing $AuCl_4^-$, and propose a synthetic route for stable metallic nanostructures with a high purity using a halogen-free Au precursor or Pt-priming. In addition, photothermal properties are proposed as a new evaluation tool for the overall structural stability of replicated metallic nanostructures. Our discovery of the role of precursor ligands in the synthesis would be highly helpful in guiding the synthesis of functional noble metal nanomaterials using silver halide templates.

Poster Presentation : **MAT.P-366**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Novel Double-Cable Polymers with Quinoxaline-Based Donor Backbone and Naphthalene Diimide-Based Pendant Acceptors

Dasol Chung, Dayeong Choi, Taiho Park[1,*]

Pohang University of Science and Technology, Korea

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

Double-cable polymer is composed of a semiconducting polymer donor backbone with acceptor pendant groups covalently connected to the polymer backbone through an alkyl bridge. The intriguing properties of double-cable polymers arise from the alkyl bridge since it is composed of single bond carbon chains. Here, a series of double-cable polymers were developed for manifold organic electronic applications. The newly synthesized double-cable polymers utilize quinoxaline derivatives as the donor backbone and naphthalene diimide (NDI) derivatives as the pendant acceptors. To inspect characteristic differences arising from the alkyl bridge, three double-cable polymers were synthesized with same quinoxaline core and NDI core but with different carbon length in the alkyl bridge varying from 6 carbons to 14 carbons. The optoelectronic and physical properties were measured through UV-vis, PL, DSC, and TGA.

Poster Presentation : **MAT.P-367**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

[Withdrawal] Enhancing Redox EC Performance through Viologen's Stable Two-Electron Transfer Reaction in Deep Eutectic Solvent

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*

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Poster Presentation : **MAT.P-368**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Three-Dimensional Gold Nanosphere heptamer for Near-Field Focusing Surface Enhanced Raman Scattering as Chemical Weapon Agent Gas Sensor

Qiang Zhao, Sungho Park[1,*]

Chemistry, Sungkyunkwan University, China
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Herein, we report the novel strategy for the synthesis of complex 3-dimensional (3D) nano structures - gold nano sphere heptamer. Briefly, we utilised platinum shell with certain thickness to prevent the nano spheres from etching. Meanwhile gold nano sphere can still maintain its localised surface plasmon resonance which is the critical core part of heptamer. Further, this core is directly grown into gold octahedron by well-faceted overgrowth followed by selective platinum deposition and gold etching to obtain platinum octahedral frame containing one nano sphere core. Finally synthesising the outer hexamer structure by octahedral frame which we reported previously to further form heptamer. The special internal nano sphere structure not only fills the inner space of hexamer, but also improves the overall electromagnetic field intensity by constructing more and dense hot spots to fully utilize whole octahedral. As expected, the core sphere greatly improves the electromagnetic field intensity and shows high sensitivity in the CEPS gas detection compared with the hexamer due to higher hot-spot. On the other hand, core sphere fills spare space existed in hexamer which provides more active attachment points for analyte.

Poster Presentation : **MAT.P-369**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nickel and Iron Ion Exchanged ZIF-67 Grown on Ni Foam for Oxygen Evolution Reaction Catalysis in Alkaline Media

Da Kyoung Jung, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Recently, there has been a growing interest in exploring alternative energy sources to replace fossil fuels because of the ongoing environmental problems caused by greenhouse gas emissions. Among these, hydrogen energy produced via water electrolysis is gaining recognition for its high energy density and lack of CO_2 emission. Metal organic frameworks (MOFs) have garnered attention as catalysts for water splitting due to their large surface areas, distinctive porosities, and crystalline morphologies. Therefore, in this work, we selected zeolite-imidazolate-67 (ZIF-67), a type of MOF, owing to its exceptional stability resulting from its unique structure comprised of Co^{2+} ions and N atoms of 2-methylimidazole. However, according to precious studies, using ZIF-67 as a catalyst alone is not favorable for oxygen evolution reaction (OER), which is the half-reaction of water splitting. Hence, we synthesized ion-exchanged trimetallic catalysts of Ni-Fe/ZIF-67/Ni foam (NF) through a simple solution process at the room temperature, looking forward to the trimetallic synergy and good stability of the substrate. The synthesized Ni-Fe/ZIF-67/NF catalysts exhibited excellent electrochemical performance for OER with an overpotential of 220 mV and stability over 100 hours without any noticeable changes at a current density of 10 mA/cm^2.

Poster Presentation : **MAT.P-370**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Hybrid MOF Structure Catalyst for Enhanced Electrochemical Performance

Hye Yeon Yoo, Min Hyung Lee[1,*]

Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

As environmental problems increase due to global warming and climate change, interest in hydrogen as an alternative energy source is increasing. However, most of current hydrogen production relies on gas reforming processes that use fossil fuels. Therefore, it is essential to develop an environmentally friendly hydrogen production method, and electrochemical water splitting is receiving great attention as one of the environmentally friendly hydrogen production methods. Oxygen evolution reaction (OER) is a half-reaction of water splitting and requires a higher overpotential than hydrogen evolution reaction (HER). Therefore, in order to realize a commercial level production of hydrogen through water electrolysis, it is essential to develop an electrocatalyst with low overpotential. Transition metal-based metal-organic frameworks (MOFs) is material with a unique porous structure and large surface area, and are being applied to various catalytic studies. In this poster, a hybrid-type structure based on two different MOFs was synthesized, and this catalyst showed improved electrochemical catalytic performances with overpotential of ~280 mV at 10 mA cm^{-2}.

Poster Presentation : **MAT.P-371**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Uniformly sized perovskite quantum dots with high PLQY enable highly efficient solar cells

Dayeong Choi, Seyeong Lim, Taiho Park[*]

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

Quantum dots are used in many applications due to their ability to control the energy bandgap according to their size. In this study, a size selection via gel permeation chromatography method was used to prepare uniformly sized quantum dots. This allows us to synthesize uniform quantum dots with high PLQY. It is significant that the problem of difficult size control during the synthesis process can be solved by obtaining uniform quantum dots through GPC after the purification process. In addition, quantum dots with narrow half-widths exhibit very small energy shifts, indicating trap-based recombination. This strategy using GPC induced the removal of small-sized particles, resulting in low energy disorder and higher power conversion efficiency than conventional solar cells using CsPbI3 quantum dots. The result was not only a high efficiency of 15.3% power conversion efficency, but also stable in a 20-day under atmospheric conditions.

Poster Presentation : **MAT.P-372**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Copper Oxalate as an Efficient Electrocatalyst for the Electroreduction of Carbon Dioxide to C2 products

Sun Mi Kim, Seon Hwa Lee, Jae Ryeol Jeong, Min Hyung Lee[*]

Department of Applied Chemistry, Kyung Hee University, Korea

In order to reduce greenhouse gas emissions and prevent climate change, the CO2 reduction reaction is an important area of research. The electroreduction of carbon dioxide into multi-carbon products in aqueous solutions is a challenging and critical process. Furthermore, the low efficiency of the production of C2 products limits performance at scale. Copper (Cu) has been widely studied for electrochemically reducing CO2 into multi-carbon (C2+) products. In this study, we synthesized copper oxalate through a simple method. The low-cost and easily synthesized copper oxalate catalyst showed high activity and excellent selectivity towards C2 products. It exhibited C2 products with a selectivity of 55.6% (faradaic efficiency) and ethylene faradaic efficiency of up to 37%. The yield of ethylene was found to depend on the reaction conditions, such as the applied potential and CO2 concentrations. These results suggest that copper oxalate is a promising candidate for large-scale CO2 reduction and the production of value-added C2 products.

Poster Presentation : **MAT.P-373**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

synthesize of $Cs_3Cu_2I_5$ perovskite single crystal

<u>Yeonju Lee</u>, Ji-Hyun Cha[1,*]

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

We successfully grew high-quality single crystals of $Cs_3Cu_2I_5$ using an antisolvent vapor-assisted crystallization (AVC) method. Millimeter-sized crystals were obtained without the need for crystal-seeding in the dimethyl formamide (DMF) solvent. $Cs_3Cu_2I_5$ single crystals were obtained at 40°C growing temperature, and polycrystals were grown at 0°C and -20°C under ambient atmosphere. Copper-based halide perovskite crystals grown in N-methyl-2-pyrrolidone (NMP) as the solvent resulted with mixed phase and small sized polycrystals. The phase purity and emission properties of the $Cs_3Cu_2I_5$ perovskite single crystals were characterized by using X-ray diffraction (XRD) and photoluminescence (PL) measurements.

Poster Presentation : **MAT.P-374**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Green-emissive copper-based perovskite quantum dots in UiO-66(Zr)

Jimin Jeong, Yeon Woo Choi[1], Ji-Hyun Cha[1,*]

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

We synthesized green-emissive copper-based perovskite quantum dots (PQDs) in UiO-66(Zr). Lead-based PQDs are efficient optoelectronic materials, but they have the disadvantage of being toxic. Recently, copper-based perovskite materials have been proposed as an alternative light-emitting material. By using metal-organic frameworks (MOFs) as a template, we synthesized stably emitting Cu-based perovskite QDs. Green-emissive PQDs@MOFs were prepared using a precursor solution in which alkali iodide and copper (I) iodide were dissolved in DMF solvent. After the precursor solution was impregnated into the MOF pores and washed with toluene solvent, yellow emission at about 600 nm was observed. When alkali iodide was added, yellow PQDs changed to PQDs@MOF with a green photoluminescence (PL) of 530 nm.

Poster Presentation : **MAT.P-375**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of all inorganic lead halide perovskites in UiO-66 MOF nanocomposite.

Minji Jeong, Ji-Hyun Cha[1,*]

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

We synthesized inorganic perovskite quantum dots (IPQDs) in a zirconium-based UiO-66 MOF. UiO-66 has a white powder, which is suitable for observing the emission color of QDs. The MOFs protected the surface of QDs and improved their stability. We impregnated a polar organic solution of PbX_2 (X = Cl, Br, I) into the pores of the MOF to prepare PbX_2@UiO-66, which was then reacted with cesium halide (CsX) dissolved in methanol. We confirmed that the PL color of $CsPbBr_3$ and $CsPbClBr_2$ perovskites in UiO-66 did not change for seven days. The compositions of the halogen anions in the perovskites can be modulated with various halide precursors, leading to $CsPbX_3$@UiO-66 composites that exhibit gradual variation of band gap energies and tuned emission wavelengths from 400 to 700nm.

Poster Presentation : **MAT.P-376**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Green and blue emissive Cs_4PbBr_6 perovskites single crystals

Chung hoe Kim, **Ji-Hyun Cha**[1,*]

Chemistry, Chungnam National University, Korea

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

We report on the optical properties of non-emissive, blue-emissive, and green-emissive Cs_4PbBr_6 perovskite single crystals. Crystals of different colors were obtained depending on the solvent and growth conditions. It is confirmed by XRD patterns that all crystals have same lattice symmetry. When synthesized in water and DMSO solvent, non-emissive crystals (WN416) and green emissive crystals (DG416), respectively, were grown. By changing the growth time in DMF solvent, we grew non-emissive (FN416), blue-emissive (FB416), and green-emissive (FG416) crystals. The band gap energies of FN416, FB416 and FG416 were measured 3.06 eV, 3.02 eV, and 2.73 eV, respectively. The PL spectrum peaks of FB416, and FG416 were observed at 497nm and 510nm, respectively.

Poster Presentation : **MAT.P-377**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Machine Learning Directed Predictive Models: Deciphering Complex Energy Transfer in Mn-doped $CsPb(Cl_{1-y}Br_y)_3$ Perovskite Nanocrystals

Hyejin Choe, **Junsang Cho**[1,*]

Chemistry, Sungshin University, Korea
[1]*School of Chemistry and Energy, Sungshin Women's University, Korea*

Machine learning(ML)-directed synthesis have emerged as a powerful tool, alternative to traditional approaches wherein a single synthetic parameter is changed at a single time along with a resulting outcome. ML approaches are more powerful, effective in not only provide a mapping of structure-function correlations but also uncovering the complex chemical reactions to reveal underlying mechanisms beyond the synthesis, which can accelerate the materials discovery. In particular, lead halide perovskite nanocrystals have recently emerged with a great potential in the photovoltaics and light-emitting didoes given their remarkable optoelectronic properties including high absorption coefficient, tunable bandgap, and nearly unitary photoluminescent quantum yield. Doping a transition metal in the semiconductor nanocrystals gives rise to an additional degree of freedom as a result of newly added optical, magnetic, and electronic properties arising from the excited state interaction between dopants and exciton. Especially, Mn2+ ions represent one of the most studied transition metal doped in semiconductor nanocrystals including lead halide perovskite, II-VI quantum dots since Mn2+ show unique emission with long-lived carrier lifetime ~ us. Understanding such effects of excited state coupling between exciton and dopants as a function of modulating the spatial distribution (concentration) and degree of coupling strength remain important. It has been reported that competitive relaxation dynamics involving the exciton and Mn energy states bring about the competing forward (from exciton to Mn) and backward (Mn to exciton) energy transfers, which in turn determine the sensitization or energy transfer efficiency. Mn2+ can potentially used as is long-lived which can be further used for carrier reservoir owing to the forbidden transition of Mn2+ (d-d). In this study, we have investigated the energy transfer mechanism in Mn-doped halide exchanged CsPb(Cl1-yBry)3 nanocrystals wherein Mn concentration and halide composition (affecting bandgap) have been systematically modulated. A machine learning directed predicted models with variety of algorithms can explore and map the multivariant design space parameters. This further enable to provide a mechanistic insight into the role of Mn concentration and electronic coupling between exciton and Mn.

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Poster Presentation : **MAT.P-378**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Li-Doping Effect on Characteristics of ZnO/rGO Micro-Supercapacitor

In Sik Lee, Min Hyung Lee*, Hye Yeon Yoo

Department of Applied Chemistry, Kyung Hee University, Korea

In recent years, micro-supercapacitors (MSCs) have attracted considerable attention in wearable and flexible micro-scale devices due to their short-charging time and high power density compared to Li-ion batteries. Despite the ongoing efforts to improve MSCs, the development of high-performance and flexible energy storage devices remains a major challenge in the field of wearable and flexible electronics. To apply MSCs for these devices, the improvement in energy density and long-term stability of MSCs are required. For enhanced capacitance of MSCs, transition metal oxides with pseudo-capacitive properties have been studied. The results of this study suggest that Li-doping of ZnO/rGO MSCs is an effective method to enhance the energy density and long-term stability of small-scale energy storage systems for wearable and IoT devices.

Poster Presentation : **MAT.P-379**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Carbon Based Bifunctional Electrocatalyst

Kang Jihun, Hye Yeon Yoo, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

The Zn-air battery has known as an energy storage device with many advantages, such as high theoretical energy density, low manufacturing cost, and stability. In the Zn-air battery, two reactions including oxygen evolution reaction (OER) and the oxygen reduction reaction (ORR) occurs simultaneously at one electrode. Until now, the expensive noble metal of Pt and Ru –based catalysts were used as the efficient catalysts for OER and ORR reactions, respectively, which requires to the development of new bifunctional catalysts to replace Pt and Ru-based catalysts. In this study, carbon-based 3D structure (Ni/C@N-CNT) was synthesized through the pyrolysis of Ni metal organic framework (Ni-MOF) and applied as the bifuntional catalyst for both OER and ORR. Ni/C@N-CNT can reach the current density of 10 mA/cm^2 at the overpotential of 328 mV for OER and show the current density of -11.3 mA/cm^2 at 0 V vs. RHE for ORR in alkaline solution. The application of Ni/C@N-CNT as bifunctional catalysts for OER and ORR opens the new approach to synthesize the metal-carbon composites to replace the noble metal-based catalysts.

Poster Presentation : **MAT.P-380**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

How Chemical Bonding Impacts Halide Perovskite Nanocrystals Growth to Bulk Films: Implication of Pb-X Bond on Growth Kinetics

Seonhong Min, Junsang Cho*

School of Chemistry and Energy, Sungshin University, Korea

Lead halide perovskites nanocrystals have emerged as a leading candidate in perovskite solar cells and light-emitting diodes. Given their favorable, tunable optoelectronic properties that is mainly tuned by modifying the size of nanocrystals, it is imperative to understand and control the growth of lead halide perovskite nanocrystals. However, during the nanocrystal growth into bulk films, effect of halide bonding on growth kinetics remains elusive. To understand how chemical bonding of Pb-X (covalency and ionicity) impact on growth of nanocrystals, we have examined two different halide perovskites nanocrystals of $CsPbCl_3$(more ionic) and $CsPbI_3$ (more covalent) derived from same parent $CsPbBr_3$ nanocrystals through post-synthetic halide ion exchanges. In-situ tracking of the growth of nanocrystals, by monitoring the spectral features of bulks (445 nm for Cl and 650 nm for I), enable us to determine the growth activation energy to be 92 kJ/mol (for $CsPbCl_3$) versus 71 kJ/mol (for $CsPbI_3$). The electronegativity of halides in Pb-X bonds governs the bond strength (150-240 kJ/mol), characteristics of bonding (ionic versus covalent), and growth kinetics and activation energies. A fundamental understanding of Pb-X bonding provides a significant insight for designing perovskite nanocrystal films with more desired optoelectronic properties.

Poster Presentation : **MAT.P-381**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Enhancing the Selectivity of the Carbon Dioxide Reduction Reaction by Controlling Ag-Decorated Cu Catalysts

Hyun-Su Kim, Min Seon Cha, Jae Ryeol Jeong, Min Hyung Lee[*]

Department of Applied Chemistry, Kyung Hee University, Korea

The tremendous use of fossil fuels since the industrial revolution has greatly contributed to global warming by producing vast amounts of CO2. To reduce our carbon footprint, one smart approach is to utilize CO2 as a source of chemical energy and feedstocks. In recent years, the electrochemical CO2 reduction reaction (CO2RR) has emerged as a promising method for converting CO2 into valuable chemicals at ambient conditions. Cu catalysts have been extensively studied for CO2RR because of their ability to produce multi-carbon products. However, the low conversion efficiency and selectivity of Cu catalysts remain significant barriers to the commercialization of CO2RR. In this study, we propose the use of Ag-decorated Cu catalysts to enhance the selectivity of C2 products. This is achieved by leveraging the conversion processes of CO2 into CO by the Ag sites and CO into C2 chemicals by the Cu sites, resulting in improved selectivity.

Poster Presentation : **MAT.P-382**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photopatternable One-dimensional Photonic Crystal Sensors for Detection of Formaldehyde and Acetaldehyde Vapors in Humid Air

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

In this study, we propose a novel method for detecting formaldehyde and acetaldehyde using one-dimensional photonic crystal (1D-PC) sensor which has alternating high-refractive-index layers (HRILs) and low-refractive-index layers (LRILs). As photo-crosslinkable HRIL and LRIL, copolymer-titania hybrid (Ti70) and aminoethyl methacrylate-based polymer (P(AEMA-co-BPA)) were synthesized, respectively, and used in fabrication of 11-layered 1D-PC sensor (Ti70/P(AEMA-co-BPA)). The 1D-PC sensor initially showed high hydrophilicity, which enables the color change of 1D-PC sensor by relative humidity (RH) induced swelling behavior. However, when exposed to the aldehydes, the 1D-PC sensor did not show any color change. This is because the primary amine groups at 1D-PC sensor reacted with the aldehydes to form imine groups which decrease hydrophilicity of the 1D-PC sensor.Peak wavelength of photonic stop band (PSB) of the 1D-PC sensor was shifted from 345 nm (RH 30%) to 720 nm (RH 80%) in pristine. However, when exposed to the aldehydes, PSB shifts of the 1D-PC sensor were significantly decreased regardless of RH. The recyclability of the 1D-PC sensor was verified through repeated five-times sensing/recovery tests using hydrochloric acid. In addition, optical properties and response rates of the 1D-PC sensor were easily controlled by changing crosslinking density through UV irradiation. Finally, we proposed potential applications of the 1D-PC sensor such as air quality monitoring sensor and security label.

Poster Presentation : **MAT.P-383**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Highly Selective rGO-In_2O_3 Sensor for the Detection of Nitrogen oxides

Deukhyeon Nam, Yoon Myung, Chan Woong Na*

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rGO-In_2O_3 hybrid materials were synthesized via a solvothermal reaction of an Indium nitrate containing rGO sheets, which were printed onto a colorless polyimide film for gas sensors. The rGO-In_2O_3 sensors showed a high response (resistance ratio = 22.3) to 500 ppb NO_2 at 150 ◦C and negligible cross-responses to C_2H_5OH, CO, NH_3, toluene, H_2, and HCHO. The enhancement of the gas sensing characteristics was attributed to the expansion of the electron depletion layer in In_2O_3 nanoparticles by forming a nano-scale p-n junction. The rGO-In_2O_3 hybrid materials on ITO/APC/ITO/CPI provides a simple and robust tool to control both the gas selectivity and the gas sensitivity.

Poster Presentation : **MAT.P-384**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

N-doped carbon black without metal as an excellent electrocatalyst for oxygen reduction reactions

Seokhyeon Jeon, Sungjin Park[1,*], Jung Won Lee

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Seokhyeon Jeon, Jungwon Lee, Junghoon Oh and Singjin Park*Electrochemical oxygen reduction reactions (ORRs) require efficient, durable, and cost-effective electrocatalysts. In this regard, the development of metal-free catalysts with excellent activity is essential. Herein we report the development of a novel two-step heating route to produce metal-free N-doped carbon blacks [1]. The prepared materials exhibit superior electrocatalytic performance for ORRs in a basic media, which is comparable to commercial Pt/C catalysts. Among the various heating temperatures tested, sequential two-step heating at 750 and 1000 °C produced the most efficient catalysts with onset and half-wave potentials of 0.97 and 0.82 V, respectively. The prepared materials show excellent selectivity for 4-electron transfer, durability, and stability in response to methanol poisoning. Control experiments using one-step heating and N-doping confirm the superiority of the two-step heating process to produce efficient electrocatalysts.Reference[1] J Oh, S Park, D Jang, Y Shin, D Lim, S Park, Carbon 2019, 145, 481-487

Poster Presentation : **MAT.P-385**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Selective synthesis of BNNT or BN-MgO hybrid structures by the control of catalyst state

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Our work reports on the successful synthesis of pure boron nitride nanotubes (BNNTs) and BN-MgO core/shell nanowires using chemical vapor deposition (CVD) with a supported catalyst. The degree of oxidation of the MgO support was found to be a key factor determining the selective synthesis of BN-MgO core/shell nanowires and BNNTs. The synthesized material was characterized through transmission electron microscopy, XRD, and thermogravimetric analysis, and its crystallinity and thermal stability were confirmed. BN-MgO core/shell nanowires showed promising neutron shielding properties and high thermal stability, suggesting their potential for use in space materials. In addition, by using a simple acid treatment method, BN fibers were obtained from BN-MgO core/shell nanowires that can be easily synthesized in large quantities and can be applied to various composite materials. CVD synthesis using supported catalysts presents a promising method for mass production of BNNTs and related materials at low temperatures.

Poster Presentation : **MAT.P-386**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Water-assisted Formation of Amine-bridged Carbon Nitride: A Structural Insight into the Photocatalytic Performance for H_2 Evolution under Visible Light

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Department of Chemistry, Inha University, Korea

Carbon nitride (C_3N_4) is a metal-free photocatalyst for H_2 production using visible light and exhibits considerable potential. Although the C_3N_4 network consists a tri-s-triazine unit structure connected by H bonds, there are several perspectives on how H bonds affect photocatalytic performance. In this study, we present a water-assisted method for the production of polymeric carbon nitride to control in-plane structures associated with H bonds and amine bridges [1]. The C_3N_4 samples manufactured by heat treatment using water and humidified air gas (CN-H) show high levels of photocatalytic activity for hydrogen evolution reactions. Structural and photophysical properties have shown that CN-H samples not only have larger domains than C_3N_4 samples produced without water (CN-A), but also have fewer H bonds and more amine bridging groups. Structural changes made through water treatment increase the in-plane migration of the photoexcited charge carriers and thus lead to improved photocatalytic performances.Reference[1] D. Jang et al. Appl. Catal. B: Environ. 2022, 310, 121313Following are results of a study on the "Leaders in INdustry-university Cooperation 3.0" Project, supported by the Ministry of Education and National Research Foundation of Korea

Poster Presentation : **MAT.P-387**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Acid-activated carbon nitrides as photocatalysts for degrading organic pollutants under visible light.

Shin Eunyoung, Sungjin Park[1,*]

Inha University, Korea
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Three-dimensional (3D) carbon nitride (C_3N_4) is a promising platform for visible-light-active photocatalysts because of its suitable band positions. This study says that HNO_3 activation improves the photocatalytic activity of 3D melamine-derived C_3N_4 (MCN) materials, which degrade the organic pollutant rhodamine B (RhB) [1]. HNO_3 treatment under reflux removes the carbonaceous impurities in MCN and introduces oxygen-containing functional groups on its surface. Under visible light irradiation, the nitric acid treated MCN (NT-MCN) completelydegrades RhB within 30 min. Photophysical characterizations and control experiments withradical scavengers reveal that MCN and NT-MCN follow different reaction mechanisms.Because NT-MCN exhibits a longer photoluminescence lifetime, smaller electrochemicalresistance, and larger photocurrent than those of MCN, it enables a better transfer of chargecarriers during the catalytic reaction.Reference[1] Haeju Kim, Dawoon Jang, Seungjoo Choi, Jeongho Kim, Sungjin ParkFollowing are results of a study on the "Leaders in industry-university Cooperation 3.0"Project, supported by the Ministry of Education and National Research Foundation of Korea

Poster Presentation : **MAT.P-388**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Control of Iron Oxide Nanocluster Size Using Solvothermal Method

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Hanbat National University, Korea

Iron oxide nanoclusters are aggregates of single iron oxide particles and exhibit unique behavior compared to single iron oxide nanoparticles. Due to its similar size to bacteria, high saturation magnetization, superparamagnetism, and low toxicity. Also it is widely utilized in various industries such as bioimaging, biosensors, and magnetic separation based on its distinctive magnetic properties that vary with size. However, there are limitations in controlling the size of iron oxide nanoclusters, such as a narrow size control range and a complicated synthesis process. To overcome this, it is necessary to study the size-controlled synthesis of iron oxide nanoclusters in a simple and wide range. In this study, the method and principle of synthesis of iron oxide nanoclusters of various sizes are presented using the solvent thermal synthesis method. By changing the synthesis factors such as synthesis time, temperature, precursor concentration, reducing agent type and concentration, the size of the iron oxide nanocluster is finely controlled between 90 and 420 nm. The size of the synthesized iron oxide nanocluster was analyzed by dynamic light scattering (DLS) and Scanning Electron Microscope (SEM) and confirmed that the particles synthesized by X-ray diffraction analysis (XRD) were Fe3O4. Through this study, we present an understanding of the synthesis factors such as reducing agent type and concentration, precursor concentration, temperature, and synthesis time, and the synthesized iron oxide nanocluster shows applicability in various fields depending on size.

Poster Presentation : **MAT.P-389**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Cesium Lead Halide Perovskite Nanocrystals as Visible-Light Photocatalysts for Stereoselective [2+2] Cycloadditions

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Semiconductor nanocrystals (NCs) has emerged as visible-light photocatalysts with several benefits, including the ability to generate charges by visible-light and transfer charges to adjacent materials, catalytic properties tunable via crystal structure modifications, and a template effect on reactants for stereoselective reactions. In this study, cesium lead halide NCs were employed as visible-light photocatalysts for stereoselective [2+2] cycloadditions. The template effect of NCs was confirmed by comparing with Ir(ppy)3 and the relationship between structure of NCs and photocatalytic activity was investigated by using NCs with different sizes and halide composition. Our results showed that the effect of quantum confinement on reaction yield was stronger than an increase in bandgap alone. Smaller NCs with the same optical bandgap showed higher yields than larger NCs, despite having smaller surface areas in contact with reactants. The effect of surface area on yield was negligible in the situation where reversible adsorption and desorption of reactants and product on the NCs surface is possible. Overall, this work provides insights into the potential of NCs as efficient and tunable photocatalysts for stereoselective reactions.

Poster Presentation : **MAT.P-390**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Study of Bi nanospheres synthesis through thermal annealing of SCC/BiOCl

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[1]*Korea Institute of Industrial Technology, Korea*

BiOCl is synthesized using the co-precipitaiton method. In this work, Bi nanospheres coated a graphene layer were synthesized by using Sodium Carboxymethyl Cellulose (SCC) in the BiOCl synthesis process. Initially synthesized BiOCl had a nanosheet structure before annealing, but changed to a ball shape after annealing in Ar atmosphere at 500 ℃. The structural properties of the sphere were analyzed by using SEM, XRD, and XPS. Also it was confirmed through raman spectra analysis that the graphene layer was coated on the sphere. The synthesized Bi spheres are expected to be used as photocatalyst.

Poster Presentation : **MAT.P-391**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Highly Enhanced Stability of Vitamin C in Nanohybrids and Its Controlled 2D/3D Structures

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Vitamin C is an essential nutrient involved in the metabolic processes of humans and plays an important role in maintaining physiological functions. It also has strong antioxidant properties. However, vitamin C is easily oxidized and decomposed when exposed to the atmosphere. The purpose of this study was to develop a stable vitamin C preparation that could be effectively used in physiological conditions for an extended period of time. To achieve this, we synthesized vitamin C-zinc basic salt (ZBS) hybrids by incorporating vitamin C into the ZBS layer during hydroxide co-precipitation. We demonstrated the change from 2D to 3D structures of the vitamin C-nanohybrids according to the concentration of ethanol in the solvent, as confirmed by Fourier transform infrared spectroscopy (FT-IR) and X-ray diffraction (XRD) analyses. We found that the vitamin C content in the nanohybrids can be altered by changing the structure of the nanohybrids, as confirmed by the ultraviolet-visible (UV-Vis) spectroscopy. Additionally, we confirmed that 3D vitamin C-nanohybrids have a high specific surface area using the Brunauer–Emmett–Teller (BET). These vitamin C-nanohybrids did not show significant cytotoxicity to fibroblasts, but showed high cytotoxicity to human melanoma and epidermal cell carcinoma. These results suggest that vitamin C-nanohybrids can stably protect vitamin C from oxidation and degradation, showing promising potential for various biomedical applications, including drug delivery.


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Poster Presentation : **MAT.P-392**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Layered Double Hydroxide-DEX Nanohybrids for Enhanced Biocompatibility

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Dexamethasone (DEX) is a type of glucocorticoid that has anti-inflammatory effects 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, DEX has limitations due to poor water solubility, which reduces its pharmacological benefits and requires higher dosages. This can lead to side effects such as osteoporosis, hypertension, peptic ulcers, hyperglycemia, and cushing's syndrome. To overcome these limitations, a drug carrier with improved efficacy for DEX is recommended. We focused on developing a new drug delivery system using layered double hydroxide (LDH) as a carrier to enhance the therapeutic potency of DEX. We used co-precipitation, ion-exchange, and exfoliation and reassembling methods to intercalate DEX into the interlayer spaces of LDH. According to X-ray diffraction, molecular spectroscopy, and thermogravimetry analyses, 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. The content of DEX in the LDH was determined by UV-vis spectroscopy. In conclusion, the DEX-LDH nanohybrid exhibited superior efficacy and improved distribution compared to DEX alone and has the potential to enhance therapeutic efficacy.


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Poster Presentation : **MAT.P-393**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Evaluating pre-clinical suitability of curcumin in exfoliated layered double hydroxide nanoparticles as lung cancer nanomedicine

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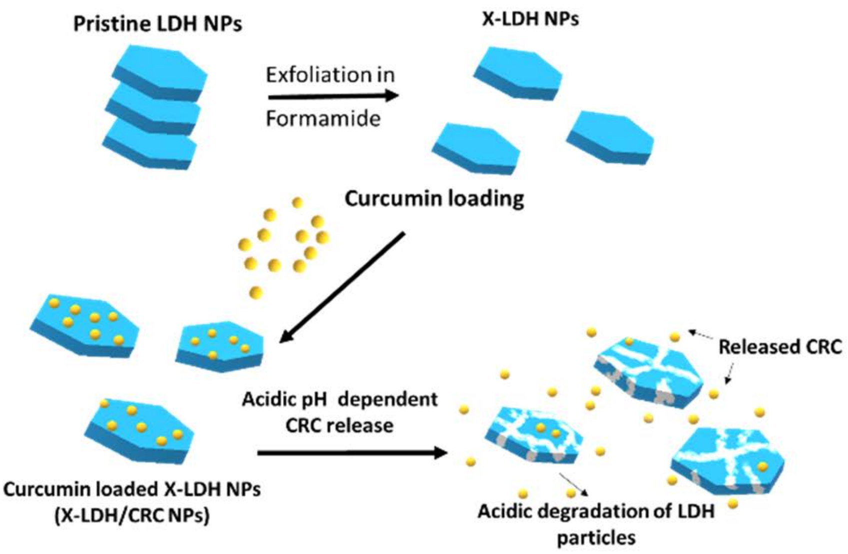
Lung cancer falls under the most threatening cancers, in terms of mortality rate, irrespective of gender and ethnicity. The most common type of lung cancer is non-small cell lung cancer (NSCLC) [1], which accounts for ~ 85 % of lung cancer incidents, whereas the small cell lung cancer (SCLC) is a rare case, which accounts for 15 % among all the cancer types that affect the pulmonary system. According to the 2021 statistics, at least 1 in every 16 Americans are diagnosed with lung cancer. In 2022 the United States is expected to have fresh cases of ~ 1.9 M with ~ 0.6 M cancer deaths, where it reports ~ 350 lung cancer mortalities every day, the leading cause of cancer death [2]. Here, we rationally designed ~ 100 nm sized curcumin (CRC) loaded exfoliated layered double hydroxide nanoparticles (X-LDH/CRC-NPs) and tested its suitability as nanomedicine in non-small cell lung cancer (NSCLC) cell lines (A549 and NCI-H460) resulting enhanced apoptosis. The preclinical evaluation on A549 tumour-bearing nude mouse model confirmed that such well-designed X-LDH/CRC NPs would be highly advantageous for treating lung cancers.Keywords: Exfoliated LDH (Layered double hydroxide), Curcumin, Lung cancer therapy, In vivo efficacyReferences1. D. I. Suster and M. Mino-Kenudson, Arch. Med. Res. 2020,51, 784.2. R. L. Siegel, K. D. Miller, H. E. Fuchs and A. Jemal, CA Cancer. J. Clin. 2022, 72, 7.


Pristine LDH NPs
X-LDH NPs
Exfoliation in
Formamide
Curcumin loading
Released CRC
Acidic pH dependent
CRC release
Curcumin loaded X-LDH NPs
(X-LDH/CRC NPs)
Acidic degradation of LDH
particles

Poster Presentation : **MAT.P-394**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

BN-CNT composite films for multi-shielding applications (EMP & Radiation)

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CNTs mat has excellent electrical conductivity, excellent mechanical properties, and especially high specific strength, so it can dramatically reduce fuel consumption when applied to the aerospace field, and can also be used as a fiber for space suits. . However, carbon nanotube mats have low oxidation resistance and no neutron shielding function, making them difficult to apply in extreme environments such as outer space. Here, boron nitride, which has high oxidation resistance and thermal neutron shielding ability, is coated to produce a carbon nanotube mat-boron nitride composite material, giving the carbon nanotube mat multifunctional and multiple shielding abilities. In the CVD process, borazine, a precursor, is thermally decomposed, and boron nitride is coated on the carbon nanotube mat to finally form a layered composite material. The thickness of the coating layer is linearly proportional to time, and the desired coating thickness can be formed by adjusting the time. The coating layer is characterized as boron nitride by the 1365 cm-1 park attributed to the E2g mode in Raman and the 1350 cm-1 (TO mode) and 780 cm-1 (R mode) peaks in FTIR. In the XPS and EELS analysis, a new C-N covalent bond was added, which means that a chemical bond was formed between the carbon nanotube mat and the boron nitride coating layer. The chemical bond at this interface means that the mat and coating layers are strongly bonded. Finally, TGA, tensile strength, and neutron shielding ability of the carbon nanotube mat-boron nitride composite were tested. As a result, the composite material showed a 190℃ increase in oxidation temperature and a 200% increase in tensile strength compared to the existing mat, and improved thermal neutron shielding performance.

Poster Presentation : **MAT.P-395**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Colloidal Tellurium Nanowire Laser in the Mid-Wavelength Infrared Region

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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) becomes narrow, and the emission intensity dramatically increases, which comes from lasing property. Surprisingly, the Te NWs exhibit the lasing within the anti-freezing solvent at ~90 K and in a human cancer cell at 78 K. It indicates the potential for realizing deep-tissue imaging and thermotherapy.

Poster Presentation : **MAT.P-396**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Molecular Simulation Study of CO_2 Cycloaddition Reaction in M-ZIF-71 (M=Zn, Co, ZnCo) with Linker Defects

SungHyun Yun, Yongchul Chung[*]

School of Chemical Engineering, Pusan National University, Korea

Chemical fixation of CO_2 with propylene oxide (PO) to produce propylene carbonate (PC) is an attractive way to convert CO_2 into valuable chemicals. Developing a catalyst that can lower the activation barrier of the ring-opening reaction for CO_2 the cycloaddition reaction can help reduce the reactor's operating cost and is a highly active area of research. Zeolitic imidazolate framework (ZIF) is a class of nanoporous material that can be used for gas separation and catalysis. Due to its topological similarity with zeolite, the material is often used for catalysis applications via catalytic active metal centers originating from framework defects. The tendency of the framework defect formation is elusive and may be related to topology and local coordination environment. In this work, we performed density functional theory (DFT) and grand canonical Monte Carlo (GCMC) simulations to evaluate the framework defect formation in a bimetallic ZIF (ZnCo-ZIF-71) to its catalytic performances for CO_2 fixation reaction. DFT calculations on Zn-/Co-ZIF-71 were performed to evaluate the activation barriers of different transition metals (M=Zn, Co) on the ring-opening mechanism for the CO_2 cycloaddition reaction. Additionally, we constructed model structures with different linker defects for M-ZIF-71 (M=Zn, Co, and ZnCo). GCMC simulations were carried out to estimate the nitrogen saturation loadings of the defective structures. By comparing the simulation and experimental data, we estimated how many linker defects exist in M-ZIF-71 (M=Zn, Co, and ZnCo), and draw a correlation between the framework defect and catalytic activity of the materials.

Poster Presentation : **MAT.P-397**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Fabrication of innocuous hydrogel scaffolds based on modified dextran for biotissues

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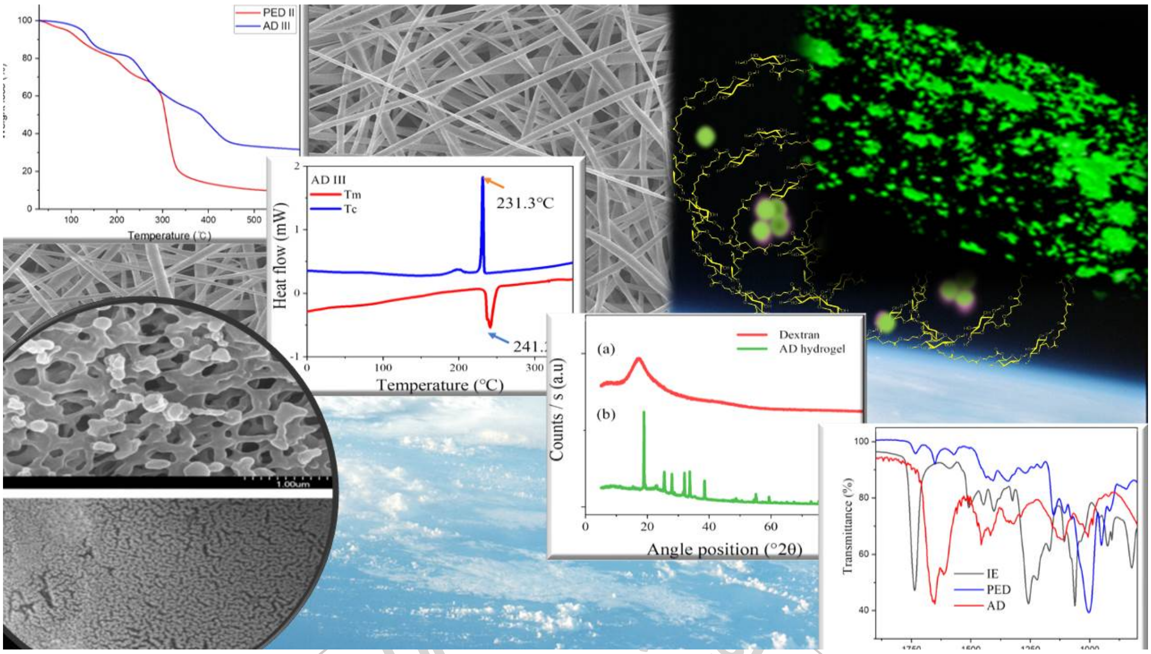
Substrates with basic structures similar to those of living tissues are useful as cellular scaffolds for the preparation of biocompatible and innocuous materials. In this study, a hydrogel matrix was prepared by introducing a functional group capable of forming crosslinks between natural polymers to create a basis for preparing a microenvironment favorable for cell adaptation. The modified dextran hydrogel polymer was designed to mimic the conditions of the extracellular matrix (ECM) as a scaffold. The precursors of the target hydrogel were synthesized using condensation with a stepwise procedure. A delicate hydrogel based on modified dextran was obtained via photo-crosslinking under room temperature at UV-254 nm. The biocompatibility of this hydrogel was verified using green fluorescence images acquired by incubating a cell line. The characteristics of the hydrogel were verified using proton nuclear magnetic resonance (1H NMR), Fourier-transform infrared (FT-IR) spectroscopy, field-emission scanning electron microscopy (FE-SEM), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), X-ray diffraction (XRD) analysis, and electrostatic spinning. The crosslinked structure and biocompatibility of the modified hydrogel were confirmed using instrumental analyses and a promising cell culture. Using TGA, the weight losses of precursor and hydrogel were determined to be 90.96% and 39.2%, respectively, up to 600 ◦C. The SEM images revealed that the surface of the modified dextran/PVA electrostatically spun fabric comprised a porous network of nanofibers from which the spheroids were entirely absent. The diameter of the fiber ranged from 200 to 500 nm depending on the electrostatic spinning. Confocal microscopy image was used to monitor the biocompatibility of this hydrogel.


PED II
AD III
100
80
60
40
20
0
100
200
300
400
500
Temperature (℃)
AD III
Tm
Tc
231.3°C
241.
Heat flow (mW)
2
1
0
-1
0
100
200
300
Temperature (°C)
1.00um
Dextran
AD hydrogel
(a)
(b)
Counts / s (a.u)
0
20
40
60
Angle position (°2θ)
Transmittance (%)
100
80
60
40
IE
PED
AD

Poster Presentation : **MAT.P-398**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Multiscale Evaluation of Xe/Kr Separation MOFs Combining Machine Learning and Process Simulation

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School of Chemical Engineering, Pusan National University, Korea

This work focuses on developing a machine-learning approach to approximate the saturation loading of adsorbent materials, which is an essential parameter for the analytical equation that is used for the process-level simulation for adsorption-based separation. Grand canonical Monte Carlo (GCMC) simulations were conducted to compute the single-component isotherms for Xe and Kr from experimental MOFs. These data were used to fit the Langmuir model equation to obtain the saturation loading parameters. We trained the machine learning (ML) model to predict saturation loading. The trained ML models were then compared with the pore volume-based approach based on the Ideal Pressure Vacuum Swing Adsorption (IPVSA) simulations. We find that the ML model is better at correctly estimating the saturation loading than the pore volume-based approach. The findings could help estimate the saturation loading parameter without calculating additional isotherm points.

Poster Presentation : **MAT.P-399**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Nicotinic Acid-Layered Double Hydroxide-Eudragit® S100 Nanohybrid as a Controlled Drug Release System

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One of the oldest extensively used hypolipidemic drugs, nicotinic acid (NA), has a variety of pharmaceutical and dermatological functions such as effective skin whitening, anti-inflammatory properties, and attenuating oxidative stress. However, the high-dosage administration of NA could lead to dermatological side effects such as flushing, erythema, and itching due to their immediate-release and fast blood clearance weakness. For this reason, it is necessary to improve the NA delivery system having controlled release property. Recently, we successfully encapsulated NA into the interlayers of layered double hydroxide (LDH) through a co-precipitation method further coated with an enteric coating agent, Eudragit® S100, for NA's slow release. According to the X-ray diffraction analysis, the basal spacing of the NA-LDH nanohybrid was determined to be 1.55 nm, indicating that the NA molecules were successfully intercalated into the interlayer space of LDH. Additionally, their particle size is around 100-200 nm based on SEM images and DLS results. The release profile in the gastrointestinal solution confirmed that NA-LDH-Eudragit® S100 nanohybrid showed sustained release property compared to rapid release NA. Also, we found that they are cyto-compatible according to the cytotoxicity data on the

L929 cell line. Therefore, we suggest that NA-LDH-Eudragit® S100 nanohybrid could be a potential controlled drug delivery system for NA molecules to have improved efficacy without any unwanted side effects.

Poster Presentation : **MAT.P-400**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Short-Wavelength Infrared Photoluminescence and Photocurrent of Nonstoichiometric Silver Telluride Colloidal Nanocrystals

Jiyeon Ban, Gahyeon Kim[1], So Young Eom, Haemin Song, Kwang Seob Jeong[*]

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

Various QDs such as HgSe, HgS, HgTe, PbSe, and PbS has been intensely investigated for the past decade in the SWIR range. However, their toxicity limits applications such as bioimaging and therapeutic use. Here, we present the nonstoichiometric silver telluride nanocrystals of Ag_xTe ($x > 2$) and Ag_2Te/Ag_2S CQDs. As the Ag/Te atomic ratio reaches 2.7, the excitonic bandgap energy can be expanded to 2.7 μm. Not only $Ag_{2.7}Te$, $Ag_{3.7}Te$ shows higher emission compared to PbSe which has intense optical properties. Ag_2Te/Ag_2S CQDs has more enhanced structural stability than the Ag_2Te core CQDs, maintaining its spherical shape under the harsh 200 kV electron beam. The reason for the improved emission property and air stability is investigated by X-ray photoelectron spectroscopy (XPS). Surprisingly, the Ag_xTe CQD film responds to the SWIR light with a responsivity of 2.1 A/W at 78 K. The optical properties and infrared photo responsibility of Ag_xTe CQDs will open various opportunities for the application of solution-based SWIR.

Poster Presentation : **MAT.P-401**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Tunable Intraband Transitions of the Self-Doped Silver Selenide Quantum Dots via Cation Exchange

Hyeong Seok Kang, Yoon Seo Jung, Haemin Song, Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

Heavy-metal free nanomaterials in the mid-infrared (mid-IR) region have been great interest in optoelectronics and bioimaging. The silver selenide colloidal quantum dots (CQDs) with the steady-state intraband transition have been known as the alternatives, but the energy range of the materials is only limited to the mid-wavelength. Here, we present the silver selenide (Ag_xSe, $x > 2$) CQDs that exhibit the intraband transitions which are produced by the cation exchange (CE) method. As the CE method preserves the size of the initial nanocrystal template , the quantum confinement effect can be maintained even after the CE process. The SWIR bandgap of the PbSe CQDs and the visible bandgap of the CdSe CQDs are successfully converted to the intraband transition of the Ag_xSe CQDs, respectively. The intraband transition of the cation exchanged-Ag_xSe CQDs are investigated by Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and spectroelectrochemistry. Also, the infrared photocurrent response of cation exchanged-Ag_xSe CQDs will provide great opportunities for the less toxic nanomaterial based-optoelectronic device.

Poster Presentation : **MAT.P-402**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Na_6ZnS_4 : Promising New Ternary Infrared Nonlinear Optical Materials

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Suncheon National University, Korea
[1] *Department of Advanced Components and Materials Engineering, Suncheon National University, Korea*

As demand for batteries with improved performance, safety, cost efficiency, and environmental sustainability increases, the development of electrolytes has become an essential factor. Among various types of electrolytes, liquid electrolytes are generally inexpensive and easy to use. However, batteries containing liquid electrolytes pose the risk of fire or explosion if damaged or overheated. In contrast, solid state electrolytes (SSEs) have lower volatility than liquid electrolytes, are thermally more stable, and can withstand high temperatures, making them a potential alternative to liquid electrolytes.Na-SSEs include sodium beta-alumina (Naβ-alumina), sodium super ionic conductor (NASICON). But there is a problem with them. So the present study is attempting to investigate Na_6ZnS_4.Na_6ZnS_4 has a hexagonal system with Na-Na distances between 3.198 and 3.416 Å, indicating possible Na conduction. However, Na_6ZnS_4 has not been considered as Na-SSEs till date. In this study, we applied various synthesis conditions (e.g., grinding methods, atmosphere, and heating/cooling protocol) to prepare phase-pure Na_6ZnS_4. It was confirmed that the most pure form was obtained by ball milling for 20 minutes and heat treating at 800℃ for 12 hours in a bowl-shaped alumina crucible. The conductivity of Na_6ZnS_4 was found to be quite low (~2 μS/cm). Since such a low conductivity is expected to be overcome by slightly adjusting the crystallographic structure, we are currently working on the effect of various dopants on the structure and ionic conduction.

Poster Presentation : **MAT.P-403**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of Metal-Boron Nitride Nanotube Hybrid Material for Potential Gamma Ray Shielding Applications

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Gachon University, Korea

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Boron nitride nanotubes (BNNTs) have gained significant attention in recent years due to their unique properties, such as high thermal conductivity, high mechanical strength, and excellent chemical stability. In this study, we synthesized a metal-BNNT hybrid material by filling WO_3 inside the BNNT, creating a composite material that combines the advantageous properties of both materials. The resulting hybrid material was characterized using various techniques, including SEM, TEM, and XRD. TEM analysis with energy-dispersive X-ray spectroscopy (EDS) mapping revealed the successful distribution of WO_3 within the BNNT, confirming the successful incorporation of WO_3 into the BNNT. Furthermore, we explored the potential of the synthesized hybrid material for gamma ray shielding applications. Our results suggest that the material has promising shielding properties, and future studies will focus on optimizing its properties for this application.

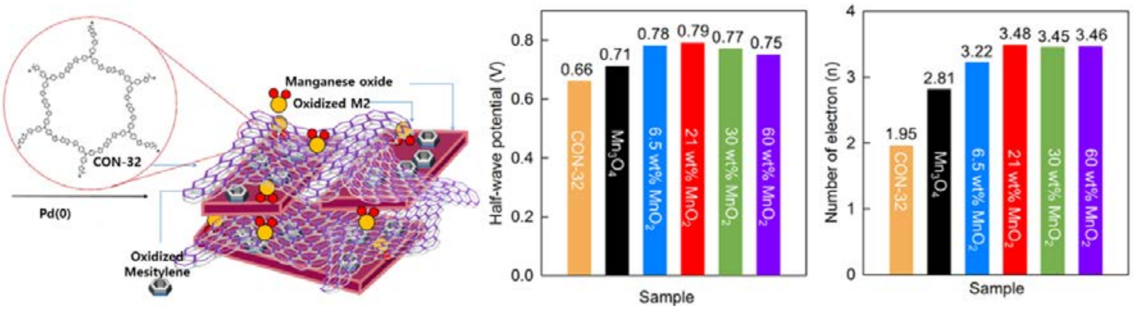
Poster Presentation : **MAT.P-404**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Redox-Based Solid Surface Interactions between Covalent Organic Nanosheets and MnO_2 for Highly Effective Oxygen Reduction Electrocatalysis

Soohyeon Park, Jin Kuen Park[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Hybridizing organic nanosheets with inorganic nanostructures has led a large amount of study attention due to its utility as an effective synthetic process for highly functional electrocatalysts. This study, a novel synthetic way to search for the potent electrocatalysts was evolved upon regulating a redox-driven intensive electronic interactions between covalent organic nanosheets(CONs), named as CON-32, and MnO_2. This synthetic method is derived from the formation of strong surface bonds like Mn-O-S and Mn-O-R, which are arised from the redox reaction between CON-32 and MnO_2. Thermal procedure on these hybrids at harsh temperatures carried to the carbonization of CON-32 and thus the advancement of electrical conductivity. Both the as-prepared and the carbonized exhibited notably enhanced electrocatalytic properties for the oxygen reduction reaction (ORR) comparing with the pristine COF, MnO_2, and Mn_3O_4, displaying a larger half-wave potential and higher electron transfer numbers being achieved; these consequences highlights the benefits of hybridization and carbonization. The important role of hybridization in upgrading the electrocatalytic features can be attributed to the outstanding improvement of the ORR kinetics together with the quick electron transfer in the boundaries of the matters to the hydroxide ions, which is arised from the synergies between conductive CONs and electrocatalytically active MnO_2, as showed by various spectroscopies.


Manganese oxide
Oxidized M2
CON-32
Pd(0)
Oxidized Mesitylene
Half-wave potential (V)
0.0
0.2
0.4
0.6
0.8
0.66
0.71
0.78
0.79
0.77
0.75
CON-32
Mn_3O_4
6.5 wt% MnO_2
21 wt% MnO_2
30 wt% MnO_2
60 wt% MnO_2
Sample
Number of electron (n)
0
1
2
3
4
1.95
2.81
3.22
3.48
3.45
3.46
CON-32
Mn_3O_4
6.5 wt% MnO_2
21 wt% MnO_2
30 wt% MnO_2
60 wt% MnO_2
Sample

Poster Presentation : **MAT.P-405**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of Aptamer-conjugated Gold Nanoparticle for Sensitive Electrochemical Detection of SARS-CoV-2 Spike Protein

Hyoung-Mi Kim, Junghun Park[1,*]

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[1]Korea Institute of Industrial Technology, Korea

The coronavirus pandemic has brought to the forefront the need for rapid, sensitive, and accurate diagnostic tests to detect SARS-CoV-2, the virus responsible for COVID-19. One promising approach is the use of aptamers, synthetic single-stranded DNA or RNA molecules that can bind to specific targets with high affinity and specificity. In this study, we developed an aptamer-based electrochemical biosensor for the detection of SARS-CoV-2 spike protein, a viral antigen commonly used in diagnostic assays, in a sandwich assay manner. The electrochemical biosensor was fabricated by immobilizing a capture aptamer onto a gold electrode and a secondary aptamer-conjugated gold nanoparticles (Apt-AuNP) was introduced to increase electrical signals. The apt-AuNP were prepared using hyaluronic acid or L-ascorbic acid, and were functionalized with the secondary aptamer containing a terminal thiol group. The Apt-AuNP properties were characterized using transmission electron microscopy, dynamic light scattering, and zeta potential measurement. The biosensor showed high sensitivity and specificity, with a detection limit of 1 pg/mL and no cross-reactivity with other respiratory viruses. The aptamer-based biosensor with the Apt-AuNP, has the potential to serve as a rapid, low-cost, and highly sensitive diagnostic tool for COVID-19, as well as for the detection of other infectious agents.

Poster Presentation : **MAT.P-406**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Microwave-Assisted Synthesis of 13C-Graphene Quantum Dots as MRI contrast agents

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

The use of contrast agents such as gadolinium is essential in Magnetic Resonance Imaging (MRI), which often causes some serious side effects including irreversible skin and organ fibrosis, and the permanent deposition in brain tissue. In particular, the use of gadolinium-based contrast agents is prohibited in patients with chronic kidney disease due to the risk of developing nephrogenic systemic fibrosis. Therefore, there is an urgent need to develop alternative MR contrast agents with less toxicity and side effects. In this study, we develop an MRI T1 contrast agent based on graphene quantum dots (GQDs) made from the source of carbon-13, a radioactive isotope of carbon with a nuclear spin of ½ that responds to nuclear magnetic resonance. To achieve this, we secure an efficient synthesis technology for 13C-GQDs and develop a purification technology to ensure their uniformity. Previously, GQDs have been mostly synthesized by a top-down approach that breaks the carbon covalent bonds of graphitic materials using heat and acid, which requires considerable time and cost to separate the GQDs from acid solvent after the synthesis. Instead, we used a bottom-up synthesis technology to produce GQDs with better biocompatibility using 13C-glucose as source materials and their hydrothermal reaction in a microwave reactor (MWR) without using acid. Finally, we confirmed excellent MRI contrast effects through in vitro MR phantom experiments, followed by in vivo experiments to verify the potential of the 13C-GQDs T1 contrast agent.

Poster Presentation : **MAT.P-407**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effect of substitution of various elements in K_3SbS_4 on ion conductivity and electrochemical stability.

Seolyeon Kang, Myoungho Pyo[1,*]

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[1]*Department of Advanced Components and Materials Engineering, Suncheon National University, Korea*

Solid-state batteries based on Li solid electrolytes (SSEs), which have been actively researched in recent years, face the problem of limited Li resources. Therefore, research on SSEs based on Na or K is expected to be an alternative that can solve this problem. In the case of Na SSE, Na_3MS_4 (M = P, Sb) is a representative compound, and it has been confirmed that ion conductivity can reach over 10 mS/cm when aliovalent doping (W^{6+}, Si^{4+}) is performed on Na_3SbS_4 to induce vacancies in the Na site. On the other hand, research on K SSEs is still in the early stages, and the only interesting research result is $K_{2.92}Sb_{0.92}W_{0.08}S_4$, which was recently reported by doping W^{6+} into K_3SbS_4. Unlike K_3SbS_4, which showed an ion conductivity of 2.5 μS/cm at room temperature, this compound exhibited a high ion conductivity of 77 μS/cm.In this research, various elements were substituted into K_3SbS_4 to investigate the effect of these substitutions on the ionic conductivity and (electro)chemical stability of the final compound. the effect of defects induced by doping some Sb^{5+} in K_3SbS_4 with W^{6+} ($K_{3-x}Sb_{1-x}W_xS_4$) on the conductivity was investigated. Currently, we are synthesizing compounds of $K_{3-x+y}(Sb_{1-x-y}W_xSi_y)S_4$ with no potassium site defects ($x = y$), compounds with vacancies ($x > y$), and compounds with interstitial defects ($x < y$). After producing the pure forms of these compounds, we plan to investigate their ion conductivity and (electro)chemical stability.

Poster Presentation : **MAT.P-408**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Transparent Luminescent Solar Concentrators Based on Copper Chloride with STE Emission and Metal Cluster Compounds.

Bobae Lee, Jun Choi, Sung-Jin Kim[1,*]

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

Luminescent solar concentrators (LSCs) are transparent solar energy harvesting systems which are able to integrate with building windows as Building integrated photovoltaic (BIPV). $Cs_3Cu_2Cl_5$ is a highly emissive material with self trapped exciton(STE) emission which has broad emission, high quantum yields(QYs), and large Stokes shifts. It also absorbs light in the UV region (no absorbance in the visible region), so it can be applied to transparent windows as an LSC material. In this work, we synthesized $Cs_3Cu_2Cl_5$ and metal cluster compounds $A_2Mo_6X_8L_6$ (A=cation, X=halogen, L=organic, inorganic ligand) and mixed them into poly(methyl methacrylate) (PMMA) waveguide to make LSCs cover broader range of solar irradiation. These eco-friendly metal halide materials as transparent and lead-free emitters for LSCs are promising as a next-generation BIPV materials.

Poster Presentation : **MAT.P-409**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

DNA-Functionalized Gold Nanoparticles for Disease Microenvironment-Responsive Photothermal Therapy

Jinseong Kim, Won jong Kim*

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

Herein, we reported rationally designed gold nanoparticles (AuNPs) decorated functional DNAs respond to disease microenvironments and disease-related factors and exhibit anti-tumor effect via photothermal therapy. AuNPs modified with two types of DNA, i-motif duplex and VEGF split aptamer, are aggregated in response to pH and formed VEGF aptamer. Thereafter, additional aggregation occurs due to the interaction between the split aptamers and the ligand while capturing VEGF, and the corresponding change results in a change in the optical properties of AuNP. According to the unique thermoplasmonic characteristic of AuNPs, when the aggregated AuNPs are irradiated with a NIR laser, heat that can show anti-tumor effects is generated. Finally, we demonstrated the enhanced anti-tumor effect of AuNPs with functional DNAs by photothermal therapy in vitro and in vivo tumor model.

Poster Presentation : **MAT.P-410**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Eco-friendly surfactant for stretchable polymeric dry adhesive epidermal electronics

Haechan Park, Kyoseung Sim[*]

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

Epidermal electronics, which are highly conformable on the skin, have significant advantages in electrophysiological monitoring and human motion sensing. Numerous approach with inorganic conductors has been developed recently, however, cost-effectiveness and biotoxicity of them are still problems. Therefore, biocompatible and cost-effective organic conductors such as poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) based composite to achieve high adhesion and stretchability have been actively investigated. Nevertheless, stretchability and adhesion are still not enough for standing movement of human body. To go beyond the limit, elastomer and organic conductor composite could be a great alternative, but only few research has been reported. Even, to blend immiscible elastomer and organic conductor, Triton X-100, which are known as toxic surfactant were used. Here, we introduce eco-friendly surfactant, Tween 80 enabled epidermal bilayer electronics which are highly stretchable, conductive, and self-adhesive. Polydimethylsiloxane (PDMS) and PEDOT:PSS were used as a elastomer, and organic conductor, respectively. Through our electronics, we could monitor long-term electrocardiography as well as human body movement.

Poster Presentation : **MAT.P-411**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Novel Anthracene HTM Containing TIPs for Perovskite Solar Cells

Sanghyun Paek[*], **Chan Woong Na**[1], **Yoon Myung**[1]

Department of Chemistry and Energy Engineering, Sangmyung University, Korea
[1]*Korea Institute of Industrial Technology, Korea*

Recently, perovskite solar cells have been in the spotlight due to several of their advantages. Among the components of PSCs, hole transporting materials (HTMs) re the most important factors for achieving high performance and a stable device. Here, we introduce a new D–π–D type hole transporting material incorporating Tips-anthracene as a π–conjugation part and di-methoxy-triphenylamine as a donor part (which can be easily synthesized using commercially available materials). Through the measurement of various optical properties, the new HTM not only has an appropriate energy level but also has excellent hole transport capability. The device with PEH-16 has a photovoltaic conversion efficiency of 17.1% under standard one sun il-lumination with negligible hysteresis, which can be compared to a device using Spiro_OMeTAD under the same conditions. Ambient stability for 1200 h shown that 98% of PEH-16 device from the initial PCE was retained, indicating that the devices had good long-term stability.

Poster Presentation : **MAT.P-412**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile strategies for the enhanced morphologies of P3HT-nanofibrils enabling high-performance soft organic transistor

Myeonghyeon Na, Kyoseung Sim*

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

Organic field-effect transistors (OFETs) have gained significant attention in organic electronics due to their potential for low-cost and stretchable electronic devices. The performance of OFETs is highly dependent on the morphology of the active material. One common material used in OFETs is poly(3-hexylthiophene) (P3HT), which can form nanofibrils (NFs) with varying microstructures depending on the solution processing conditions. This study investigates the effect of solution-dependent modification of P3HT-NFs morphology on the performance improvement of OFETs. We modified the morphology of P3HT-NFs using a facile cycling fibril formation process. We found that longer P3HT-NFs resulted in higher mobility, a measure of the transistor’s ability to conduct electrical current. Furthermore, the OFETs with longer P3HT-NFs showed a lower threshold voltage and higher on/off ratio, indicating improved transistor performance. In conclusion, we demonstrate the importance of controlling the morphology of the active material in soft OFETs, highlighting the potential for improving OFETs' performance.

Poster Presentation : **MAT.P-413**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of a Ferritinophagy-Assisted Ferroptosis-Inducing Agent for Improved Anticancer Therapy through a pH-Responsive Drug Release Platform

Junha Lim, Won jong Kim[1,*]

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

The use of ferroptosis-based therapy as a potential treatment for cancer has gained significant attention. However, the effectiveness of this therapy is often limited by the redox system specific to cancer and the presence of ferritin, which acts as a storage site for iron ions. To address this limitation, we developed a novel agent called the PUS complex, which utilizes a pH-responsive drug-releasing platform. The platform is made by polymerizing phenylboronic acid and decorating it with iron oxide, making it easily loaded with sulfasalazine through interaction with PBA. The PUS complex can release sulfasalazine in response to the acidic pH of lysosomes in cancer cells and degrade into labile iron ions (Fe2+). This process inhibits the production of GSH and induces an improved ferroptosis anticancer effect through the facilitated Fenton reaction. Notably, the PUS complex has demonstrated the ability to effectively regress tumors in in vivo models, highlighting its potential as a solution for iron-based therapeutics through simultaneous ferritinophagy-ferroptosis events.

Poster Presentation : **MAT.P-414**
Material Chemistry
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigation of Calcium-ion Insertion and Extraction Mechanism in Titanium 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 titanium 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 180 mAh/g. 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-415**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Study on the Synthesis of High-Purity Mg(OH)2 using Bittern with dolomite

Yeong Jo Yun, Jae Wook Jung, Yoojin Kim[1,*]

Engineering Materials Center, Korea Institute of Ceramic Engineering and Technology, Korea
[1]*Engineering Materials Center, Korea Institute of Ceramic Engineering and Technol, Korea*

High-purity hexagonal plate Mg(OH)2 was synthesized by using bittern and dolomite. Mg(OH)2 powder can be obtained by separating Ca ions in bittern with CaSO4 using H2SO4 and then refining them. Purification technology and pH control is important because Ca ions must be removed in the bittern for high purity Mg(OH)2. To reduce the production cost of Mg(OH)2 we adopted calcinated dolomite (dolime). Controlling the ratio of dolime and NH4OH was an important key for purity. Synthesized Mg(OH)2 was characterized by Inductively Coupled Plasma (ICP) and X-Ray Fluoresce (XRF).

Poster Presentation : **MAT.P-416**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

One step SiO2 Coating Process of ceramic pigments

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Korea Institute of Ceramic Engineering and Technology, Korea

[1]*Engineering Materials Center, Korea Institute of Ceramic Engineering and Technol, Korea*

To improve the physical properties and applications of ceramic pigments. SiO2 coating is important. The SiO2 coating improves color, prevent agglomeration at high temperatures. Synthesis of red-yellow pigment FeOOH, and addition of Tetraethyl orthosilicate(TEOS) for silica coating proceed in a basic condition. In addition, we focused on synthesizing and coating pigments in one precess. The pigments are synthesized using a hydrothermal reactions, and the synthesized solution is subjected to silica coating after TEOS is added in a basic catalytic atmosphere without a purification process. Silica-coated nanopowders were characterized by transmission electron microscope (TEM), UV-vis, and CIE lab. As a result of the analysis for confirming silica shell.

Poster Presentation : **MAT.P-417**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Amorphous Quaternary Sulfide Compound for Solid-state Electrolyte

Yuna Kim, Sung-Jin Kim[1,*]

chemistry & nano science, Ewha Womans University, Korea
[1]*Department of Chemistry, Ewha Womans University, Korea*

All solid state electrolyte batteries is the core of the development of electric vehicle technology and is the most important material technology to secure high density, large capacity, and stability of batteries. Since safety devices such as cooling device and separators are not required, cost reduction. In addition, a high capacity is possible because lithium metal with a superior capacity compared to graphite can be used as an anode. In this work, amorphous sulfide compound $LiSbGeS_4$ was designed and synthesized by aliovalent substitution so that there is a cationic defect in the Li $M(III)S_2$ structure of the 3D three-phase sulfur compound Li-M-S system. $LiSbGeS_4$ characterized by PXRD, Raman and XPS to analyze the local structure of amorphous material. In addition, an anionic-substituted compound was synthesized to improve the lithium-ion conductivity, and oxysulfide was synthesized by substituting a small amount of oxygen in place of sulfur to increase the air stability. Li-ion conductivity was measure by electrochemical impedance spectroscopy (EIS) analysis.

Poster Presentation : **MAT.P-418**

Material Chemistry

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Aqueous monomethylmercury degradation using nanoscale zero-valent iron through oxidative demethylation and reductive isolation

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[2]*Department of Civil and Environmental Engineering, Nazarbayev University, Kazakhstan*
[3]*ENVIRONMENTAL, GIST, Korea*

This paper proposes a Fenton-like reaction activated by nanoscale zero-valent iron (nZVI) for aqueous mono- methylmercury (MMHg) decomposition. Reacting 10 μg L− 1 MMHg with 280 mg L− 1 nZVI removed 70% of the aqueous MMHg within 1 min, and its main product was aqueous Hg(II). Within 1 − 5 min, the aqueous Hg(II) decreased while the aqueous, solid, and gas-phase Hg(0) increased with 92% MMHg removal. Then, a secondary Hg(II) reduction to solid Hg(0) was prevalent within 30 − 60 min, with 98% MMHg removal. Diverse-shaped magnetite crystals were observed on the surface of nZVI in 2 h, suggesting that Fe(II) oxidation on magnetite can be a source of electrons for secondary Hg(II) reduction. When FeCl2 and H2O2 were added to the MMHg solution without nZVI, 99% of the MMHg changed to Hg(II) within 1 min. The reactive oxygen species (ROS) produced by the Fenton-like reaction accounted for the rapid demethylation but not for the further reduction of Hg(II) to Hg(0). The results suggest a three-step pathway of MMHg decomposition by nZVI: (1) rapid MMHg demethylation by ROS; (2) rapid Hg(II) reduction by Fe(0); and (3) slow Hg(II) reduction by magnetite on the nZVI surface.

Poster Presentation : **ELEC.P-425**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Controlling ion pairing for shifting redox potentials and enhancing the stability of naphthalene diimide in non-aqueous redox flow batteries

Seongmo Ahn, Hye Ryung Byon[*]

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Here, we demonstrated naphthalene diimide (NDI) and Li^+ coupled electron transfer in acetonitrile (MeCN). The NDI is an excellent model for the stepwise two-electron transfer process. Its low solubility by the strong π-stacking interaction was surmounted by introducing ammonium cationic substituents to the NDI via simple condensation and N-alkylation. As a result, two ammonium-tethered NDI and bistriflimide ($TFSI^-$) as the counter anion showed 0.9 M solubility in MeCN. Two cathodic events made an anionic radical and dianionic NDI core, respectively. The received electron is delocalized over the NDI core and also stabilized by pairing it with the cation. Cyclic voltammograms showed ~120 mV of potential difference from two cathodic waves with Li^+ of LiTFSI electrolyte in MeCN, which was narrower than ~370 mV with K^+ of KTFSI. It suggested that the Li+ possessing high charge density was closely coupled with the anionic radical NDI, expediting the second electron-transfer process. The process was also dependent on non-aqueous solvents. High donor-number (DN) solvents widened the potential difference with Li^+ because a thick solvation shell of Li^+ weakened the ion coupling. We applied this system for non-aqueous RFBs. Unlike two distinct galvanostatic plateaus appearing with K^+, the ammonium-introduced NDI with Li^+ showed almost a single overlaid plateau caused by the rapid reduction of the anionic radical. The ammonium-tethered NDI/Li^+ in MeCN cells performed high cyclability and low crossover through an anion exchange membrane, showing a capacity fading rate of 0.0089% for 1000 cycles in RFBs.

Poster Presentation : **ELEC.P-426**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Determining the Depolymerization of Super-Engineering Polymer By using Simple and Rapid Electrochemical Methods

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Mechanical properties and processability of a polymer highly depend on molecular weight. Therefore, controlling the depolymerization of a polymer in storage is a major concern for polymer synthesis and application. The molecular weight of polymers is determined by viscosity measurements, gel permeation chromatography (GPC), and nuclear magnetic resonance (NMR) spectroscopy. However, those methods generally require large amounts of polymer samples and relatively long measurement times, and some polymers are continuously decomposed after the polymerization is finished. So, due to the difficulty of analyzing polymer depolymerization with conventional methods, we need a new analysis method. In this presentation, we demonstrated a new simple electrochemical method based on cyclic voltammetry for measuring the depolymerization of the polymer during polymer synthesis. As the molecular weight of the polymer decreases due to thermal depolymerization, the viscosity of the corresponding polymer solution is decreased. Thereby, the diffusion of redox species is not disturbed, resulting in a proportional increase in steady-state current. By drawing a calibration curve of current versus thermal depolymerization time for a polymer, we can determine the molecular weight tendency of the polymer in solution more easily and instantly than by using conventional methods. Based on this research, we can expect that it will be possible to precisely analyze polymer depolymerization in a short time. In addition, this electrochemical method requires short measurement time and small sample sizes, which show great potential for analyzing and maintaining the properties of polymers in industries.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ELEC.P-427**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Rugged forest morphology of magnetoplasmonic nanorods for photoelectrochemical water splitting

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

A feasible nanoscale framework of plasmonic heterogeneous materials and proper surface engineering can enhance photoelectrochemical (PEC) water-splitting performance owing to increased light absorbance, efficient bulk carrier transport, and interfacial charge transfer. Here, a new magnetoplasmonic Ni-doped Au@FexOy nanorods-based material is introduced as a novel photoanode for PEC water splitting. The core-shell Ni/Au@FexOy MagPlas NRs were synthesized by a two-step process, i.e., one-pot solvothermal synthesis of Au@FexOy, where the hallow FexOy nanotubeareis a hybrid of Fe2O3 and Fe3O4 and its sequential hydrothermal treatment for Ni doping. Then, a transverse magnetifield-induceded assembly was adopted to decorate Ni/Au@FexOy ofluorine-dopeded oxide glass to be an artificially roughen morphologic surface, called rugged forest, which allows more light absorption and electrochemical active sites. Then, for charactering its optical and surface properties, COMSOL Multiphysics ssimulationsre carried out. The core-shell Ni/Au@FexOy MagPlas NRs has achieved a photocurrent of 2.72 mA·cm-2 at 1.23 VRHE benefiting from the rugged morphology that provides more active sites and oxygen vacancies as the hole transfer medium, and high scattered light absorption to improve the interface charge transfer performance of the photoanode. It is probable that the current observation provides important insights about plasmonic photocatalytic hybrids as well as surface morphology into the fabrication of efficient photoanodes for PEC.

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Poster Presentation : **ELEC.P-428**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of Sb_2Se_3/MXene@NC Anode for High-Performance Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) have an increasing demand as a main power supply for large-scale energy storage and electric vehicles. Graphite has been mainly used as an anode in LIBs. However, because of its low theoretical capacity of 372 mAh g^{-1}, metal selenides are currently attracting attentions as anode materials to replace graphite. Especially, Sb_2Se_3 has been considered as an anode material in LIBs due to its high theoretical capacity of 670 mAh g^{-1}, as well as high natural abundance and chemical stability of the constituent chemical components. However, Sb_2Se_3 undergoes considerable volume expansion during cycling, which can deform the structure of the electrode. Furthermore, Sb_2Se_3 suffers from low electrical conductivity, resulting in poor cycling performance. A novel Sb_2Se_3/MXene@NC (Sb_2Se_3/MX@NC) composite was synthesized to tackle these problems. The electrostatic attraction between negatively charged MXene and positively charged Sb^{3+} can make Sb_2Se_3 particles homogenously distributed on the surface of MXene, which can enhance mechanical stability, electrical conductivity, and flexibility of the Sb_2Se_3 electrode. Therefore, the Sb_2Se_3/MX@NC composite showed the improved structural stability and superior cycling performance compared to bare Sb_2Se_3.

Poster Presentation : **ELEC.P-429**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of SnSe@N-Doped Graphitic Carbon by Cation Exchange Reactions for a High-Performance Anode in Lithium-Ion Batteries

Na Hyun An, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Lithium-ion batteries (LIBs) are the most popular energy storage system due to their relatively high energy and power density. Graphite, mainly used as an anode in commercial LIBs, is inexpensive and has stable cycle performance, but gives a low theoretical capacity (372 mAh g^{-1}). Metal selenides have been extensively researched as an alternative to graphite owing to their high theoretical capacity and electrical conductivity. In particular, SnSe is a promising candidate due to its high theoretical capacity of 847 mAh g^{-1}, chemical stability, and natural abundance. However, it suffers from large volume changes and aggregation during cycling, leading to rapid capacity fading and low specific capacity. To address this issue, N-doped graphitic carbon coated SnSe (SnSe@NGC) was synthesized using a cation exchange method. The SnSe@NGC showed a discharge capacity of about 1066 mAh g^{-1} after 100 cycles at a current density of 0.2 A g^{-1} in the voltage range of 0.01-3.0 V, which is superior to that of bare SnSe (about 309 mAh g^{-1}).

Poster Presentation : **ELEC.P-430**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

FeOF Nanorod Doped with Ni as a Cathode for Enhanced Sodium-Ion Battery Performance

Boram Yun, Jongsik Kim*

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Sodium-ion batteries (SIBs) have emerged as an alternative to lithium-ion batteries because of their abundant reserves of sodium and low cost. Recently, intercalation-type materials such as $Na_3V_2(PO_4)_3$, $Na_7V_3(P_2O_7)_4$, and $NaFePO_4$ have been studied as a cathode for SIBs, but the theoretical capacities of these materials are limited to less than 150 mAh g^{-1}. In contrast, iron oxyfluoride (FeOF) has a high theoretical capacity of 885 mAh g^{-1}, offering promise as a cost-effective cathode material for SIBs. However, FeOF suffers from poor cyclic stability and low rate performance due to low electrical conductivity and slow ion diffusion. To solve these problems, we attempted to synthesize FeOF with Ni doping ($Fe_{1-x}Ni_xOF$) to improve its structural stability and electrochemical property. The $Fe_{0.99}Ni_{0.01}OF$ electrode had a reversible discharge capacity of 450.4 mAh g^{-1} at 100 mA g^{-1} and a low fading rate of 0.21 % per cycle after 100 cycles in the voltage range of 1.2-4.0 V. In addition, $Fe_{0.99}Ni_{0.01}OF$||hard carbon in a full cell showed a high energy density of 876.8 Wh $kg^{-1}_{cathode}$ with a power density of 172.8 W $kg^{-1}_{cathode}$ and a voltage range of 1.0-4.0 V, showing the potential as a high-performance cathode material for SIBs.

Poster Presentation : **ELEC.P-431**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of Dye-Sensitized Photo-Rechargeable Flow battery for indoor light harvesting

So Yeon Yoon, Deok-Ho Roh[1], Tae-Hyuk Kwon[1,*]

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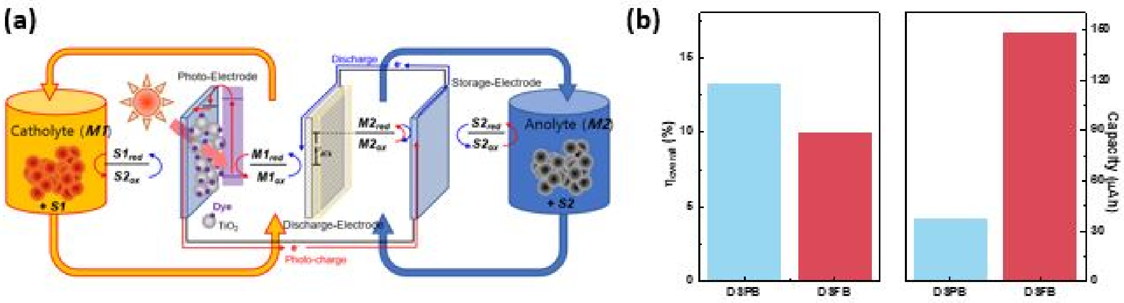
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

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[1],[2], and the efficiency achieved about 10 %. Reference[1] Energy Environ. Sci. 2020, 13, 1473-1480[2] ACS Energy Lett. 2021, 6, 1198-1204Figure 1 (a) Schematic figure of structure of DSFB (b) The result of overall efficiency and capacity



Poster Presentation : **ELEC.P-432**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Stable plating and stripping of sodium metal anodes for all-solid-state batteries enabled by an artificial bromide-based solid electrolyte interface

Manasi Mwemezi, Myoungho Pyo[1,*]

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Earth-abundant metal anodes are desirable for the development of both high power and energy density secondary storage devices. Due to the increased safety issues arising from batteries utilizing liquid-electrolytes, all solid state batteries have of recent gained more attention because of their potential to improve battery safety and energy density. Sodium metal is a promising anode material because of its high abundance and low cost. However, sodium metal is very challenging to use because it has a tendency to react with the electrolyte which limits stable cycling performance. In this study we establish a bromide-based solid electrolyte interface (SEI) on the sodium metal surface that enables stable cycling of Na|Na_3SbS_4|Na symmetric cells over prolonged hours. The use of this artificial film helps to mitigate these challenges by suppressing rapid continuous growth of solid-electrolyte interphase (SEI) and promoting stable plating and stripping of sodium metal at room temperature.

Stable plating and stripping of sodium metal anodes for all-solid-state batteries enabled by an artificial bromide-based solid electrolyte interface.

*Manasi Mwemezi, and Myoungho Pyo**

Abstract

Earth-abundant metal anodes are desirable for the development of both high power and energy density secondary storage devices. Due to the increased safety issues arising from batteries utilizing liquid-electrolytes, all solid state batteries have of recent gained more attention because of their potential to improve battery safety and energy density. Sodium metal is a promising anode material because of its high abundance and low cost. However, sodium metal is very challenging to use because it has a tendency to react with the electrolyte which limits stable cycling performance. In this study we establish a bromide-based solid electrolyte interface (SEI) on the sodium metal surface that enables stable cycling of sodium|Na_3SbS_4|sodium symmetric cells over prolonged hours. The use of this artificial film helps to mitigate these challenges by suppressing rapid continuous growth of solid-electrolyte interphase (SEI) and promoting stable plating and stripping of sodium metal at room temperature.

Poster Presentation : **ELEC.P-433**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Si Microparticles within Wrinkled-Multilayered-Graphenes for High-Areal-Capacity Lithium-ion Batteries

InCheol Heo, Jaeseong Kim[1], Sangyeop Kim[1], Won Cheol Yoo[2,*]

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Even nanostructured Si electrodes have demonstrated stable electrochemical performances in lithium-ion batteries (LIBs), complex process and high-cost of nanostructured Si electrodes are far from industry standards. Thus, utilization of commercially available low-cost Si microparticles with high-performance is highly necessary for high-energy-density LIBs. In this presentation, we demonstrate a simple and scalable method to utilize commercially available Si microparticles (ca. 7 μm) with wrinkled-multilayered-graphenes (Si-WMGs) for high-areal-capacity LIBs. The WMGs provide not only mechanical flexibility for mitigating large volume change of Si microparticles during deep charge/discharge processes, but also good adhesion property to effectively coalesce Si microparticles, and high electrical conductivity, resulting in binder- and conductor-free thick electrodes. The Si-WMG electrodes showed high initial areal capacities of 12.5 mAh cm^{-2} at 0.1 C and 7.1 mAh cm^{-2} even at a very high rate of 2 C, with outstanding long-term stability with 5.3 mAh cm^{-2} at 2 C for over 240 cycles. Furthermore, a full cell composed of Si-WMG and lithium cobalt oxide presented 3.13 mAh cm^{-2} and a stable cycling performance (90.3% retention after 100 cycles) in a practical cell setting, clearly demonstrating the practical applicability of Si-WMG electrodes. Therefore, the WMG as a binder and conductor could be applicable to other electrodes with a large volume change and high mass-loading for high-areal-capacity LIBs.

Poster Presentation : **ELEC.P-434**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Adsorption Modes of Gold Nanoclusters onto TiO_2 Modulated by pH and Cations

Jin Ho Bang[*], Minwook Jeon[1]

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[1]*Applied Chemistry, Hanyang University, Korea*

Investigating the interface of metal nanocluster (NC)-sensitized photoelectrodes is of great importance for understanding the unique photoelectrochemical (PEC) properties of NCs. Since the electrostatic adsorption of NCs on TiO_2 can create many surface states, the adsorption process can have a critical influence on the charge transfer mechanism in the NC-TiO_2 system. However, the understanding of the adsorption process and its impact on PEC behavior is very limited to date. In this work, we revealed that there are various binding modes between NCs and TiO_2, which are governed by the pH of a sensitization solution and the presence of different cations. This new insight is crucial for the development of the NC-TiO_2 system because the PEC behavior of NC-TiO_2 photoelectrodes is intimately altered by even a subtle change in the interface.

Poster Presentation : **ELEC.P-435**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Manganese Suppresses the Memory Effect of $LiFePO_4$

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[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Recently, $LiFePO_4$ (LFP) has attracted great attention as an alternative to Ni-based cathode materials because of its excellent stability. However, many obstacles remain for the widespread use of LFPs in a variety of applications. One of the problems with LFP is the memory effect, which is an unusual electrochemical behavior stemming from a previous charge/discharge history. This can be detrimental because it is difficult to determine the exact state of charge during battery operation. Our recent study showed that partial replacement of Fe by Mn can dramatically suppress the undesirable memory effect of LFP. The underlying reasons for this suppression and its impact on battery performance are discussed.

Poster Presentation : **ELEC.P-436**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Low-Content Ir Catalyst Synthesized Using NaCl Template for Efficient Proton Exchange Membrane Water Electrolysis

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

Decades of fossil fuel use have caused significant environmental pollution, which has prompted the development of new alternative energy sources. Hydrogen has been considered as the most promising energy carrier because of its high gravimetric energy density. Specifically, water electrolysis (WE) techniques can produce hydrogen without any carbon emissions. Among the WE techniques, proton exchange membrane water electrolysis (PEMWE) has been extensively investigated because of its high performance, compact design, and fast response to fluctuating loads. However, as PEMWE proceeds under acidic conditions, the catalyst selection is limited to precious metal. In this regard, developing low-content precious metal catalyst is the most suitable solution to reduce the overall cell stack price of PEMWE and realize its practical implementation. In this presentation, we suggested a synthesizing strategy for tin oxide-supported iridium oxide (IrO_x/SnO_y_NaCl) catalyst by utilizing grinded NaCl as a sacrificial template for oxygen evolution reaction (OER), which is the sluggish anode reaction of PEMWE. Combined analysis based on electrochemical and X-ray spectroscopic characterizations showed that the use of NaCl template optimized the electronic structure of IrO_x/SnO_y and reduce Ir particle size, to be beneficial to OER. Accordingly, IrO_x/SnO_y_NaCl catalyst showed a high OER activity and mass activity, comparable to those of the state-of-the-art Ir-based OER catalysts. Moreover, it showed a high single-cell performance for PEMWE, in particular, achieving 2.6 times higher mass activity than that of commercial IrO_2.

Poster Presentation : **ELEC.P-437**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Molybdenum oxide decorated carbon nanotube composite as electrode material for enhancing supercapacitor performance

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

Compared to other energy storage devices, supercapacitors have advantages such as fast charge-discharge rate, excellent energy density, high power density and long cycle life. However, the inherently low energy density of supercapacitor limits its widespread commercial application. MoO3 is a highly attractive supercapacitor electrode material because of its diverse metal oxidation states, relatively low cost and environmentally friendly properties. However, the inherent limited conductivity of MoO3 causes a large deviation from theoretical capacity in actual energy storage applications. To overcome this problem, we prepared Molybdenum oxide decorated carbon nanotube composite (MoO3-CNT) nanocomposites in the presence of thiolated CNTs by the sol–gel method. The prepared nanocomposite was characterized by XRD, XPS, and TEM. the electrochemical performance of the MoO3-CNT nanocomposite was evaluated with the cyclic voltammetry for the electrode material in supercapacitors

Poster Presentation : **ELEC.P-438**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Carbon dot-incorporated MoFe catalysts for N_2 reduction toward NH_3 electrosynthesis under ambient conditions

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Department of Chemistry, Daegu University, Korea

Nanostructured molybdenum-iron incorporated with carbon dots coated carbon cloths (CD-MoFe/CC) were produced for ammonia electrosynthesis through nitrogen reduction reaction (NRR) under ambient conditions. The catalytic NH_3 yield for NRR was measured using a gas-tight H-type cell separated by a Nafion membrane in electrolyte purged with high purity N_2 (or Ar) gas. The prepared catalysts were characterized by a broad range of analytical techniques to elucidate their physico-chemical properties confirming structural features. Optimal catalyst composition (3:1 mol ratio of Mo and Fe precursors) can provide sufficient active sites to react with target species and enhance the interaction between active sites and the adsorbed N_2 species. The CD-MoFe/CC achieved a high activity, which was superior to that of reported MoFe-based catalysts. To verify that the ammonia is produced from NRR electrocatalyzed by CD-MoFe/CC, comparative experiments were also carried out. For example, the electrolysis of 0.1 M PBS with continual N_2 bubble is conducted at an open circuit potential. There is negligible disturbance on NRR performance from supplying gas and atmosphere. The bare carbon cloth exhibits very little detection of NH_3. This work provides us an attractive catalyst material for efficient NH_2 electrosynthesis.

Poster Presentation : **ELEC.P-439**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

ZIF-derived ZnCo nanoparticles as efficient electrocatalyst for oxygen reduction reaction

Sojin Jung, Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Bimetallic zeolite imidazole framework (ZIF) materials exhibit highly attractive properties and have drawn increased attention. In this study, a novel ZnCo-ZIF has been constructed by a involved mixing of metal precursors and proper agents into a solvent. It was observed that the ZnCo-ZIF catalysts with controlled molar ratios of zinc and cobalt precursors had distinctly different effects on the morphology of single metal ZIF and its catalytic activity for the oxygen reduction reaction (ORR). Several characterization techniques such as SEM, TEM-EDX, XRD and XPS were applied to confirm that the structure formed possesses a high nano-crystallinity and porosity with a large surface area. The catalytic activity for ORR was examined using linear-sweep voltammetry and rotating ring-disk electrode techniques. The ZnCo-ZIF catalysts exhibited high catalytic activity and stability during ORR in an alkaline environment compared to their counterparts. A quantitative estimation of the electron transfer number per dioxygen molecule involved in the ORR and peroxide formation by two-electron reduction of O_2 was estimated through the disk and ring currents. The n value of ZnCo-ZIF for the ORR was over 3.5 and the yield of peroxide was below 20.0% at +0.4 V (vs. RHE). This work provides a highly efficient and affordable electrocatalysts for ORR, which may have practical application in fuel cells.

Poster Presentation : **ELEC.P-440**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nanoscale Heterostructure Interfacial Condition for High-Energy All-Solid-State Batteries

Sungwon Hwang*, **Song Junehyeok**[1]

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Recently, the use of stable lithium nanostructures as substrates and electrodes for secondary batteries can be a fundamental alternative to the development of next-generation system semiconductor devices. However, lithium structures pose safety concerns by severely limiting battery life due to the growth of Li dendrites during rapid charge/discharge cycles. For the development of next-generation system semiconductor devices, solid electrolyte nanostructures, which are used in high-density micro-energy storage devices and avoid the instability of liquid electrolytes, can be promising alternatives for next-generation batteries. Nevertheless, poor lithium ion conductivity and structural defects at room temperature have been pointed out as limitations. This study applied a low-dimensional GQD layer structure to demonstrate stable operation characteristics based on Li+ ion conductivity and excellent electrochemical performance. Transmission electron microscopy was performed to elucidate the Li+ ion mechanism of action in the modified GQD/electrolyte heterostructure. The low-dimensional structure of GQD-based solid electrolytes can provide an important strategy for stable scalable solid-state power system semiconductor applications at room temperature. A full Li GQD-based device was fabricated to demonstrate the practicality of the modified Li structure using the Li-GQD heterointerface. This study promises that the low-dimensional structure of Li-GQDs can be an effective approach for the stabilization of solid-state power system semiconductor architectures. ※ This work was supported by the International Science & Business Belt support program, through the Korea Innovation Foundation, funded by the Ministry of Science and ICT.

Poster Presentation : **ELEC.P-441**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Systematic Analysis of Degradation Features in Proton Exchange Membrane Water Electrolysis under Renewable Energy-Mimicking Fluctuating Loads

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[1]*Center for Hydrogen·Fuel Cell Research, Korea Institute of Science and Technology, Korea*
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With the intensification of the hydrogen economy, cost reduction in manufacturing and operation becomes a significant challenge for proton exchange membrane water electrolysis (PEMWE). Given that the current hydrogen strategy focused on renewable energy sources (RES) coupling and the electrolyzer capacity growth, precise estimation of durability in RES-coupled PEMWE and development strategy for durable materials are the major challenges. However, there is a lack of systematic study for a fundamental understanding of degradation features in PEMWE, especially under RES-mimicking fluctuating loads. In this work, a set of stability tests including high-resolution “real-like” solar profile, steady-state, and dynamic profiles were introduced, and the corresponding degradation features were intensively analyzed. The applied “real-like” solar profile featured a high resolution of 1 second, which allows it to reflect high ramp-rate events of RES. Diverse degradation features, including membrane degradation, catalyst dissolution and migration/diffusion, and Ti porous transport layer passivation, were scrutinized along with the dynamic of electrochemical properties. The results of the “real-like” solar profile were featured by activation overpotential recovery during “night time” periods, elevated fluoride release rate, and Pt dissolution/diffusion. Among applied profiles, the steady-state profile at elevated load and dynamic profile with cycling from 5 % of nominal to elevated load jointly mimic the solar profile-derived degradation features. The obtained results give valuable insight to bridge the gap between laboratory-scale investigation and on-site PEMWE-ReS operation and derive a rational guideline for developing an accelerated stress test protocol with combined load patterns.

Poster Presentation : **ELEC.P-442**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Transition metal phosphate on ternary transition metal sulfide to applied all-solid-state hybrid asymmetric supercapacitor

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The supercapacitor is one of the traditional energy storage devices. Supercapacitors are divided into two main categories based on the operating principle: electrochemical double layer capacitor (EDLC) which stores charges through the electrochemical double layer generated on the electrode surface and pseudocapacitor which stores charges through the redox reaction of material on the electrode surface. Herein, we prepared the ternary transition metal layered double hydroxide (LDH) and sulfide on nickel foam by the hydrothermal and galvanic exchange. And last, electrodeposited cobalt phosphate (CoP_x) was grown on the surface of ternary transition metal sulfide (t-TMS) for applied constant current density, and we denoted it as CoP_x/t-TMS/NF. Morphology and crystallinity of CoP_x/t-TMS/NF was checked by FE-SEM, FE-TEM, XRD, and FT-IR. As prepared CoP_x/t-TMS/NF and activated carbon on NF (AC/NF) was applied to the positive and negative electrodes of the hybrid asymmetric supercapacitor, respectively. It exhibits a wide potential window, enough high energy and power density, and long-term stability. The combination of nanosize CoP_x particle and 2-D structure of the nanosheet array of t-TMS indicated the high electrochemical performance.

Poster Presentation : **ELEC.P-443**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Application of Multidimensional 0D CsPbBr3 Perovskite Quantum Dots on 3D MAPbI3 Layered Structure to Perovskite based Solar Cells

Gayoung Seo, Seong Yeon Park, Jo Hyeonyeong, Taeyeon Kim, Seog Joon Yoon*

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Since after early 21st century, researchers have been devoted themselves to the ABX3 (A = MA+, FA+, and Cs+, where MA+ : methylammonium, FA+ : formamidinium, B = Pb2+ and Sn2+, and X = Cl-, Br-, and I-) perovskites to apply to solar cells, so the photoconversion efficiencies of the perovskite based solar cells have been exceeded to 25% recently. The detailed interfacial kinetics, coverage, and stability were studied but still the imperfect coverage of the hole transport materials (e.g. Spiro-OMeTAD) induced the humidifying of the perovskite so device stability was negatively affected. In this study, we introduced multidimensional 0D CsPbBr3 perovskite quantum dots on 3D MAPbI3 layered structure to modify the hydrophilicity of the perovskite surface, and to prevent the direct contact in between the perovskite film and humidity. We performed various photoelectrochemical studies to elucidate the role of perovskite quantum dot coverage to the photoconversion efficiencies of the perovskite-based solar cells and their stabilities.

Poster Presentation : **ELEC.P-444**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Multidimensional 0D CsPbBr3 Perovskite Quantum Dots on 3D MAPbI3 Layered Structure to Modify Photophysical Properties and Hydrophilicity.

Taeyeon Kim, Jo Hyeonyeong[1], Gayoung Seo[1], Seong Yeon Park[1], Seog Joon Yoon[2,*]

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The ABX3 (A = MA+, FA+, and Cs+, where MA+ : methylammonium, FA+ : formamidinium, B = Pb2+ and Sn2+, and X = Cl-, Br-, and I-) perovskites have been proposed their potentials by applying them to optoelectronic devices and solar driven chemistry. By controlling the growth kinetics, the multidimensional (0D dots, 1D rods/wires, 2D sheets/plates, and 3D bulk layered structures) perovskites has been widely studied about their material/photophysical/electrochemical properties. However, comparing to the fast electron transfer kinetics, the hole transfer kinetic regime is slower than the electron transfer kinetic rate. Also, about the interfacial contact to the hole transport materials (e.g. Spiro-OMeTAD, PTAA, etc.,), the imperfect contact and coverage lead to induce the humidity-induced perovskite hydrate formation, with also inducing the lost of photophysical properties of the perovskites. In this study, by covering the 0D CsPbBr3 perovskite quantum dots (PQDs) on the 3D MAPbI3 bulk layered structure, the interfacial contact and the material stability were improved. Surrounded by long carbon chain ligands, the PQD spin-coating process was able to introduce hydrophobic nature on the hydrophilic perovskite bulk film. This study can provide the role of interfacial hydrophilicity to the material/photophysical natures of the perovskites.

Poster Presentation : **ELEC.P-445**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Improvement of a Synthetic Strategy to Enhance Dispersity of Perovskite Quantum Dots in Various Solvents for Higher Emission Quality with Wide Color Gamut

Seong Yeon Park, Gayoung Seo, Jo Hyeonyeong, Taeyeon Kim[1], Seog Joon Yoon[2,*]

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Three-dimensionally confined ABX3 perovskite (A = MA+, FA+, and Cs+, where MA+: methylammonium, FA+: formamidinium, B = Pb2+ and Sn2+, and X = Cl-, Br-, and I-) quantum dots (PQDs) has been utilized to various optoelectronic devices and solar driven chemistry due to their outstanding photophysical properties. So far, numerous efforts have been made to improve the synthetic strategy to reduce the energy payback time for practical applications. One of them, the ligand-assisted reprecipitation process was introduced to synthesize the PQDs under ambient condition at room temperature but there were negative aspects, such as lower photoluminescence quantum yield, aggregation with lower dispersity in numerous organic solvents, and so on. In this work, by introducing as long carbon chain ligands (oleylamine and oleic acid) into the synthetic process, highly dispersed PQDs were obtained in various organic solvents. In addition, by applying the halide exchange process, the wide color gamut was also obtained. This study could be utilized to the display industry to reduce pixel size for higher brightness with wide color gamut.

Poster Presentation : **ELEC.P-446**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Incorporated B-site metal in the CsPbBr3@SiOx core-shell perovskite quantum dots to elucidate their photophysical properties.

Jo Hyeonyeong, Gayoung Seo, Seong Yeon Park, Seog Joon Yoon*

Department of Chemistry, Yeungnam University, Korea

ABX3 perovskite has been extensively studied in various fields such as ferroelectronics, actuators, sensors, and current solar power chemistry. In the early 21st century, organometallic halide perovskites were widely used in solar cells by improving its performance by up to 25.2%. Changing multidimensional perovskite also opens up more flexible applications such as photocatalysis, CO2-reduced quantum dot light-emitting diodes, etc.,. To commercialize various perovskites, it is very necessary to shorten the energy recovery time, improve the performance of perovskite-based devices, increase the stability to H2O and O2, and reduce the toxic elements. Various efforts have been utilized to replace environmentally toxic elements to eco-friendly element. In this study, we developed a synthetic strategy under ambient condition at room temperature to replace toxic Pb to Cu in the core-shell perovskite quantum dots and their materials and photophysical properties.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ELEC.P-447**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Determining Electrochemical Properties of β-FeSe Using Cyclic Voltammetry

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PbO type FeSe is a well-known as superconducting material, whereas FeSe quantum dots are reported as typical semiconductors in recent studies. As iron selenide compounds have both superconductivity and semiconductivity depending on their size and structure, we expect that β-FeSe will also have property of either one. In this research, we conducted experimental studies of β-FeSe with particular attention to the electrochemical properties. Cyclic voltammetry was used to see the redox reactions and to verify the redox potential change in different kinds of electrolytes and electrodes. The changes in β-FeSe band gap due to the changes in electrochemical properties were also analyzed. Two different kinds of electrolyte solutions- aqueous and organic solvents were used, while glassy carbon and FTO(Fluorine-doped Tin Oxide) electrodes were used as working electrodes.

Poster Presentation : **ELEC.P-448**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

In-Situ Growth of Ultrathin NCM-P Nanosheet on ZIF-derived Porous Co_3O_4 Scaffolds for Flexible Asymmetric Supercapacitor

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Phosphorus compounds, such as metal phosphides and phosphates exhibit excellent performances and great potential in electrochemical energy storage. Herein, we report the fabrication of transition metal phosphate electrodes (PANI@Co_3O_4@NCM-P) on carbon cloth through a multistep method, containing Zeolitic imidazolate framework (ZIF)-templated thermal annealing and electrodeposition. With a polyaniline (PANI) nanolayer as the interlayer, a ZIF-L array structure was well-deposited on the carbon cloth surface. The porous Co_3O_4 scaffolds were obtained by thermal treatment of ZIF-L templates in air. Then, ultrathin NiCoMn-P nanosheets (NSs) were in-situ electrodeposited on the surface of Co_3O_4 array, constructing a hierarchical structure. Benefiting the unique hierarchical structure, high conductivity of Co_3O_4 array core and large surface area of NCM-P NSs shell, the CC@PANI@Co_3O_4@NCM-P electrode exhibits excellent electrochemical properties, such as high specific capacitance of 4.5 F cm^{-2} at a current density of 1 mA cm^{-2}, and good rate capability. Furthermore, the solid-state hybrid asymmetric supercapacitor (SHAS) device with PVA-KOH gel electrolyte displays a maximum specific capacitance of 1.1 F cm^{-2} with 0.391 mWh cm^{-2} energy density at 1.66 mW cm^{-2} power density and exhibits 89% capacitive retention. Therefore, the strategy of constructing core-shell structure based on MOF templates could be extended to other electrochemical fields.

Poster Presentation : **ELEC.P-449**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Interface engineering of TMDs and CoP heterostructure on Carbon cloth for highly efficient hydrogen evolution reaction

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2D transition metal dichalcogenides (TMDs) are known as alternative electrocatalysts for hydrogen production due to their high catalytic activity, low cost, and easy preparation. Recently, transition metal phosphides (TMPs) are efficient semiconductor materials in hydrogen evolution reaction(HER) and desulfurization (HDS) which have high stability and electrically conductivity due to their low bandgap. Especially Co-based phosphides have been widely used in the HER due to their highest activity among the TMPs. However, the still limited catalytic activity compared to precious metal electrocatalysts in alkaline condition means that the development of new catalysts is needed. This work reports the possibility of designing novel and efficient HER catalysts by combining the promising CoP and TMDs. Also, Carbon cloth substrate takes advantage of high catalytic activity of TMDs with high conductivity, flexible surface. Herein, we synthesized a novel HER hybrid catalyst that is constructed by simple growth of TMDs and CoP on the surface of Carbon cloth. The synthesized TMD-CoP on the carbon cloth required low overpotential 60.7mV to approach 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 : **ELEC.P-450**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Atomic Level Study on CO_2-to-CO Electroreduction Catalyzed by Atomically Precise Bimetallic Nanoclusters

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Electrocatalytic CO_2 reduction reaction (CO_2RR) is an efficient way of converting CO_2 into high-value chemicals. Even though many metal nanocatalysts were used as CO_2RR electrocatalysts, understanding structure-property relationships still remains challenging due to their polydispersity in sizes, shapes, and surface structures. Here, I present the identification of active sites for the CO_2RR using atomically-precise bimetallic nanocluster series - $Ag_4Ni_2(SR)_8$, $Ag_4Pd_2(SR)_8$, $Ag_4Pt_2(SR)_8$, where SR is a thiolate ligand. Nanoclusters can be prepared in molecularly pure forms with crystallographically determined structures, so structure-property relationships can be studied clearly. To identify the active sites, the CO_2RR activities of bimetallic nanocluster series and Ag nanocluster were compared through electrochemical experiments using the flow-cell system. By conducting loading effect test, the active sites for CO_2RR catalyzed by bimetallic nanocluster series were experimentally identified. Moreover, although metal-doped Ag nanocluster series have very similar crystal structures, they showed different CO_2RR and hydrogen evolution reaction(HER) activity depending on the doped metal. Among the bimetallic nanocluster series, $Ag_4Ni_2(SR)_8$ exhibited the best CO_2RR activity and as the atomic number of doped metal increased, CO_2RR activity decreased. Finally, in contrast to the trend of CO_2RR activities, HER activities during CO_2RR of the bimetallic nanocluster series showed the opposite trend.

Poster Presentation : **ELEC.P-451**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Development of high-energy lithium-sulfur batteries via redox-active interlayer strategy

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Lithium-sulfur batteries have theoretical specific energy higher than state-of-the-art lithium-ion batteries. However, from a practical perspective, these batteries exhibit poor cycle life and low energy content owing to the polysulfides shuttling during cycling. To tackle these issues, researchers proposed the use of redox-inactive protective layers between the sulfur-containing cathode and lithium metal anode. However, these interlayers provide additional weight to the cell, thus, decreasing the practical specific energy. Here, we report the development and testing of redox-active interlayers consisting of sulfur-impregnated polar ordered mesoporous silica. In this case, interestingly, sulfur storage/trapping occur at the polar silica while electron transfer at conducting agent in pOMS/S_x IL during charge-discharge. Differently from redox-inactive interlayers, these redox-active interlayers enable the electrochemical reactivation of the soluble polysulfides, protect the lithium metal electrode from detrimental reactions via silica-polysulfide polar-polar interactions and increase the cell capacity. Indeed, when tested in a non-aqueous Li-S coin cell configuration, the use of the interlayer enables an initial discharge capacity of about 8.5 mAh cm^{-2} (for a total sulfur mass loading of 10 mg cm^{-2}) and a discharge capacity retention of about 64 % after 700 cycles at 335 mA g^{-1} and 25 °C.

Poster Presentation : **ELEC.P-452**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Ionic conductors exhibiting strong interaction with a polymer matrix under high temperatures and non-humidified conditions

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PA-PBI membranes are used as PEMFC polymer electrolyte membranes operating under high temperatures and non-humidified conditions. However, since the interaction between PA and PBI is weak, a large amount of phosphoric acid leaks during PEMFC operation. In this study, to solve the phosphoric acid leakage problem, we developed new ionic conductors that do not leak even under high temperatures (~200 °C) and non-humidified (RH 0%) conditions. As a result, polyphosphoric acids and phosphoric acid-based ionic liquids were selected as candidates to replace phosphoric acid. Polyphosphoric acids were expected to form strong ionic interactions with ammonium ion groups of polymer electrolyte membranes to suppress leakage of phosphate groups and improve ionic conductivity. In addition, phosphoric acid-based ionic liquids were expected to prevent phosphoric acid leakage by improving the matrix's polarity. We fabricated the polymer electrolyte membranes by doping the discovered ion conductors into an ammonium ion-based polymer matrix. As a result, the polymer electrolyte membranes exhibited excellent ionic conductivity and durability at 0% RH and 200 °C. In this presentation, we will explain the synthesis strategy and the mechanism of ionic conductivity enhancement.

Poster Presentation : **ELEC.P-453**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

New Highly Graphitized N-Doped Carbon as a Robust Supports for Pt Fuel Cell

Muhammad Irfansyah Maulana, DongHyun Lee, Jong-Sung Yu*

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

For polymer electrolyte membrane fuel cells (PEMFCs), the state-of-the-art electrocatalysts are based on carbon-supported Pt group metals. However, current carbon supports suffer from carbon corrosion during repeated start-stop operations, causing performance degradation. We report a new strategy to produce highly graphitized carbon with controllable N-doping that uses low-temperature synthesis (650 ℃) from g-C_3N_4 carbon-nitrogen precursor with pyrolysis using Mg. The high graphiticity is confirmed by high-intensity 2D Raman peak with low I_D/I_G (0.57), pronounced graphitic XRD planes, and excellent conductivity. Without further post-treatment, this highly graphitized N-doped carbon (HGNC) material combines high pyrrolic-N content with high porosity. Supporting Pt on HGNC exhibits excellent oxygen reduction activity for PEMFC with greatly improved durability as proved by real-time loss measurements of Pt and carbon, the first to surpass the DOE 2025 durability targets for both catalyst and support. The Pt/HGNC prepared at 650 ℃ shows 32 and 24% drop in mass activity after accelerated durability tests of both electrocatalyst and support, respectively, which are less than DOE target of 40% loss. The atomistic basis for this durability is explained via quantum mechanics-based molecular dynamics simulations. Interestingly, it is found that pyrrolic-N strongly interacts with Pt, making the Pt catalyst more stable during fuel cell reaction. We expect that high porosity robust graphitized materials will lead to many other novel applications for electrocatalysis with durable carbon frameworks.

Poster Presentation : **ELEC.P-454**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

IrO_2-ZnO Composite Oxide Lotus-Root-like Multichannel Nanotube as an Enhanced Electrocatalyst for pH-Universal Oxygen Evolution Reaction via Morphological and Crystallographic Control

Yoonhee Nam, Dasol Jin, Chongmok Lee[1], Youngmi Lee[*]

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Hydrogen is an excellent candidate as clean and sustainable energy source to reduce the dependency on traditional fossil fuels. Electrochemical water splitting, which involves hydrogen evolution reaction (HER) on cathode and oxygen evolution reaction (OER) on anode, is a promising strategy for hydrogen production. However, OER is kinetically challenging due to its sluggish mechanism with complex four proton-coupled electron transfer process, and therefore impedes overall water splitting. In this respect, a rational design (e.g., controlled morphology, porosity and crystallinity) for efficient OER electrocatalysts is significantly important. Herein, IrO_2-ZnO composite oxide lotus-root-like multichannel nanotubes are synthesized via electrospinning and subsequent calcination. The variation of morphological and crystallographic properties is controlled via different blending ratio of two polymers in the electrospinning solutions. Physical characteristics of the surface morphologies and elemental compositions are investigated by field-emission scanning electron spectroscopy (FE-SEM) and transmission electron microscopy (TEM). The crystalline structures are analyzed through high-resolution X-ray diffraction (XRD). Thermal behaviors for the synthesized nanomaterials are investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) method. Electrochemical measurements focused on OER performance are carried out with rotating disk electrode (RDE) voltammetry under pH-universal conditions. 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).

Poster Presentation : **ELEC.P-455**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Iridium Diphosphide (IrP_2) Nanoparticles for Electrochemical Sensing of Hydrogen Sulfide

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Hydrogen sulfide (H_2S) gas can be released from industrial activities, for example, coal gasification and refining of crude oil, and can also be generated through natural biological processes such as decomposition. But H_2S is highly toxic and flammable gas capable of causing serious health problems, including respiratory failure, nervous system damage and even death. Therefore, monitoring the levels of H_2S is important in preventing harmful impacts on human health. Various methods have been reported for detecting H_2S, including gas chromatography and fluorescence. Among them, electrochemical sensors are particularly advantageous for H_2S detection due to their simplicity and capability of real-time direct analysis. In particular, amperometric sensors generally have high sensitivity and fast response time, making them useful for detecting low concentrations in real-time. Herein, we synthesize iridium diphosphide (IrP_2) nanoparticles by acid/base precipitation and thermal annealing process. Synthetic conditions such as annealing atmosphere and temperature are controlled to alter crystalline phase of synthetic materials. Physical properties are analyzed by field-emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM). Electrocatalytic performances of synthetic materials are evaluated with cyclic voltammetry and amperometry in neutral solution to figure out their activities toward H_2S oxidation. 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).

Poster Presentation : **ELEC.P-456**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Iridium-Molybdenum Mixed Oxide Nanomaterials for Highly Performed Oxygen Evolution Reaction in a Wide Range of pH

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As the needs for carbon-neutral energy in modern society have increased, it is significant to develop sustainable and environment-friendly energy generation. Electrochemical water splitting including oxygen evolution reaction (OER) is one of methods to produce hydrogen fuel, an attractive alternative to fossil fuels. OER accompanies four electrons/protons coupled for the reaction and demands high overpotential to overcome the kinetic energy barrier. Accordingly, many studies have been conducted to exploit efficient and low-cost electrocatalysts for OER. Here, we suggest the synthetic strategy and physical/electrochemical characterization of iridium-molybdenum mixed oxide nanomaterials as highly efficient electrocatalysts for pH-universal OER. $Ir_xMo_{1-x}O_y$ nanomaterials are synthesized via electrospinning and following calcination process by controlling the metal molar ratio. The morphology and catalytic activity have been varied depending on the atomic ratio of Ir/Mo. The morphology and composition of the synthesized materials are characterized by a field-emission scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HRTEM) and X-ray photoelectron spectroscopy (XPS). Their crystalline structures are investigated through X-ray diffraction (XRD). Electrochemical measurements of $Ir_xMo_{1-x}O_y$ nanomaterials are performed with rotating disk electrode (RDE) voltammetry in Ar-saturated pH-universal aqueous solution to evaluate OER performances. 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).

Poster Presentation : **ELEC.P-457**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Perovskite $BaIrO_3$ Nanofibers for Being Applied for Potentiometric pH Sensing

Subin Choi, Hee Ah Oh[1], Myung Hwa Kim[2], Youngmi Lee[*]

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As pH is related to a lot of information such as water quality and health conditions, accurate measurements of pH are greatly demanded. Glass electrodes have been commonly for pH sensing used due to their good sensitivity, stability, and selectivity. However, glass electrodes have various problems including alkaline errors. Thus, the fabrication of new materials has been investigated to make improved pH electrodes. Particularly, iridium oxide (IrO_x) is considered as an alternative material due to various advantages like wide pH range sensing and less chemical interference. However, for the economic aspect, reducing the content of noble metals (e.g., Ir) should be considered while improving performance.In this work, we introduce perovskite $BaIrO_3$ nanofibers as an enhanced potentiometric pH sensing material in a wide pH range upto extremely basic conditions. $BaIrO_3$ nanofibers were synthesized via electrospinning and calcination processes. The morphology of $BaIrO_3$ nanofibers was measured by field-emission scanning electron microscopy (FE-SEM). The physical property of $BaIrO_3$ 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 $BaIrO_3$ 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).

Poster Presentation : **ELEC.P-458**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Potential-Dependent Mass Transport in Hydrophilic and Hydrophobic Nanochannels

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Vertically aligned nanochannel membranes have attracted attention in various applications such as sensors, energy conversion and storage, and biomimetic devices. We fabricate pH-sensitive nanochannel membranes composed of block copolymers (BCP), i.e., polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP), on planar gold electrode by spin coating method. The membrane exhibits anion-selective character at pH < pK_a of P4VP (~4.8), resulting from protonation at the pyridine nitrogen atom. Conversely, the BCP membrane becomes hydrophobic and charge-neutral at pH > pK_a due to the deprotonation at the pyridine. These pH-dependent hydrophobic and hydrophilic reversal behaviors are electrochemically monitored. When a sufficiently negative potential is applied to the gold electrode, e.g., $E < -0.8$ V, a strong electric field exerted into the nanochannels induces electrowetting switching from the dewetted state, allowing the mass transport of redox species to the electrode. In the present study, electrowetting and dewetting reversible behaviors in the nanochannels are investigated as a function of pH and electric potential.

Poster Presentation : **ELEC.P-459**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Nobel hydrophilic co-polymer mediator for enhancing the blood glucose meter (BGM).

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In this study, a new hydrophilic polymer, Poly(vinylimidazole-co-imidazole acrylic acid) P(VI-co-IA), was synthesized by co-polymerization of the 1-vinylimidazole and 4-imidazole acrylic acid for enhancing the blood glucose meter (BGM). The Os(bpy)2Cl2, a transition metal complexes which was synthesized between osmium and bipyridine ligand, were coordinated with hydrophilic polymer. The chemical properties of new mediator was confirmed by FT-IR, UV-Vis, and 1H-NMR. And their electrochemical characterization were measured by Cyclic voltammetry, multi-potential step, and zeta potential. Furthermore, the response to glucose were checked by cyclic voltammetry and amperometric I-T curve using FAD-GDH. Lastly, the interference effects of endogenous substances, such as uric acid, ascorbic acid, serotonin, and dopamine, were examined to confirm the specificity of the glucose sensor. The results showed that the P(VI-co-IA)-Os(bpy)2Cl2 complex had potential as a glucose sensor for blood glucose meter (BGM).

Poster Presentation : **ELEC.P-460**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Synthesis of polymer coordinated mediator for development of glucose dehydrogenase (GDH) enzyme electrode for efficiency of the mediator electron transfer (MET) system

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In this study, we concentrated to observe the mediator which can transfer the electron from glucose to the electrode by glucose dehydrogenase. The hydrophobic Poly(4-vinylpyridine) was quaternized with 2-Bromoethanol to synthesize a hydrophilic polymer, which has a molecular weight around ~MW 160,000 and ~MW 60.000. The electrochemical properties of the synthesized PVP(Q)-OH-Os(dmo-bpy)2Cl2 complex were determined by cyclic voltammetry (CV), multi-potential step, zeta potential, and amperometric I-T curve. The structural properties of a mediator were confirmed by UV-vis, FT-IR, SEM, and 1H-NMR. For comparing the efficiency of the mediator electron transfer, we fabricated electrodes immobilized glucose dehydrogenase (GDH) with PVP(Q)-OH-Os(dmo-bpy)2Cl2, which has different molecular weights. Finally, the electrochemical sensitivity were carried out by CV, multi-potential step, and amperometric I-T curve. Therefore, our PVP(Q)-OH-Os(dmo-bpy)2Cl2 complex showed good performance as an anode electrode for using glucose sensor and biofuel cell.

Poster Presentation : **ELEC.P-461**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Improving solubility and stability of the polymer coordinated mediator for continuous glucose monitoring (CGM)

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In this study, we improved an enzyme-based glucose sensor to enhance the solubility and stability for continuous glucose monitoring (CGM). We synthesized Os(dmo-bpy)2Cl2 by coordinating 4,4'-dimethoxy-2,2'-bipyridine(dmo-bpy) ligands onto osmium, a transition metal element. We also synthesized PVI-HEA(Poly vinylimidazole-Hydroxyethyl acrylate) by copolymerising 1-vinylimidazole and 2-hydroxyethyl acrylate to provide high solubility and stable fixation ability. And then, we synthesized PVI-HEA-Os(dmo-bpy)2Cl2 which has various ratio between 1-vinylimidazole and 2-hydroxyethyl acrylate (1:1, 2:1, and 4:1). And, the synthesized mediator was characterized by H-NMR, UV-Vis, FT-IR, and SEM. Additionally, electrochemical properties were carried out by cyclic voltammetry, multi-potential step, and amperometric I-T curve to check the quantitative amount of glucose. Also, we confirmed the electrochemical interfering effects in vivo substances such as ascorbic acid, uric acid, dopamine, and serotonin. Finally, our electrode showed long term stability and the potential for application of the continuous glucose monitoring (CGM) systems.

Poster Presentation : **ELEC.P-462**
Electrochemistry
Exhibition Hall 2+3 (1F) THU 11:00~13:00

Enhanced Ethylene Selectivity in Electrochemical CO_2 Reduction Reaction through Control of Planarity in Molecular Copper Complexes.

Dongho Seo, **Ki Min Nam**[*]

Department of Chemistry, Pusan National University, Korea

In recent years, research into carbon dioxide (CO_2) conversion technologies has been actively pursued due to the sharp increase in atmospheric CO_2 concentration. Among them, electrochemical CO_2 reduction technology has garnered attention as an environmentally friendly technology that can safely process CO_2 and convert it into useful energy. However, the problem of multi-carbon product selectivity in CO_2 electrochemical reduction technology still remains a challenge. To address this issue, we conducted a study to increase the selectivity of multi-carbon products in CO_2 electrochemical reduction reactions using a copper organometallic catalyst with phenanthroline ligands. We confirmed that the selectivity of multi-carbon products increases in the presence of copper clusters, and that the selectivity of ethylene (C_2H_4) increases as the planarity of the complex increases. Moreover, when the complex is immobilized onto a carbon support, we found that not only does the current density increase, but the generation of methane (CH_4), a C1 product, is suppressed, leading to a maximum C_2H_4 selectivity of up to 30%. These results are expected to provide an important foundation for improving the performance of CO_2 electrochemical reduction technology using copper organometallic catalysts and enhancing the selectivity of multi-carbon product formation.

Poster Presentation : **ELEC.P-463**

Electrochemistry

Exhibition Hall 2+3 (1F) THU 11:00~13:00

Electrochemical Nitrate Reduction to Ammonia on Cobalt Catalysts

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The electrochemical conversion of nitrates to ammonia recycles the fixed nitrogen and offers an attracting and supplementary alternative to the energy- and resource-intensive Haber-Bosch process. It is also valuable to remove the nitrates, a widespread nitrogen pollutant, for water treatment. However, this conversion not only involves the complicated eight-electron reduction to transform nitrate into ammonia but simultaneously suffers from the competitive hydrogen evolution reaction and other nitrate reduction pathways, challenged by a lack of efficient catalysts. Recent studies have shown that oxygen vacancies of oxide catalysts can adjust the adsorption energies of intermediates and affect their catalytic performance. Among various explored nitrate reduction catalysts, cobalt shows great potential due to its intrinsic selectivity to ammonia and high efficiency. In this study, the CoO/Co composite electrode was successfully synthesized by using the CoO nanostructures deposited on the Co plate. The obtained CoO/Co composite electrode was applied to the electrochemical nitrate reduction reaction, and this electrode exhibited dominant ammonia selectivity and durability due to the interfacial coupling effect.

Poster Presentation : **EDU.P-419**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Implications of the Phase Diagram in the 2015 Revised Chemistry II Textbook

YoungHa Hwang, Seounghey Paik*

Department of Chemical Education, Korea National University of Education, Korea

In this study, six types of 2015 revised curriculum Chemistry II textbooks were analyzed for conditions, definitions, whether or not critical points were displayed, and real-life examples of phase diagram. In this study, it was confirmed that the problems pointed out in several previous studies were not reflected in the 2015 revised curriculum Chemistry II textbook. The same as the situation defining the phase diagram, the translation of the phase diagram into a phase equilibrium diagram, the distinction between phase and state being unclear, the critical point not being shown in the phase diagram, real life examples are very limited what is being presented as is suggested as a problem. Therefore, it is necessary to reflect the results of various previous studies in the revised curriculum Chemistry II textbook that will be made in the future, specify the conditions under which the phase diagram is drawn, newly model the situation defining the phase diagram, and translate the phase diagram as a ‘phase diagram’. It is necessary to use the term, clarify the distinction between phase and state, mark the critical point in the phase diagram, and develop various real-life examples.

Poster Presentation : **EDU.P-420**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Analysis of chemistry domain in new elementary science textbooks for 5th and 6th grade

Young Tae Kong

Science Education, Chinju National University of Education, Korea

n this study, in order to derive the implications necessary for the application of the newly revised 2022 science curriculum to the school, an analysis of the contents of the chemistry domain was conducted among elementary school science textbooks (for 5th and 6th grade).The subjects of the study were 7 books published in 2023, and government-issued textbooks (for 5th and 6th grade) published in 2019 were added for comparison. The analysis framework [1] was divided into 1) external comparison of textbooks, 2) composition of chemistry section, 3) advanced science content, and 4) science reading and story.As a result of the analysis, compared to the national science textbooks, the newly compiled science textbooks presented various advanced science contents and materials in advanced science and science reading and story, and provided sufficient career guidance such as job introduction.However, since these textbooks are based on the 2015 science curriculum, there was no significant change in the composition of differences in the chemistry area compared to the national science textbooks.[1] Young-Tae KONG (2022). A comparative study of the contents of chemistry domain in the new elementary school science textbooks for grade 3 and 4. 130th General Meeting of the Korean Chemical Society. 130(1), 149.This research was partially supported by the National Research Foundation of Korea (2016R1D1A1B02008712).

Poster Presentation : **EDU.P-421**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The affective effect of coteaching to the pre-service teachers in overseas educational volunteer activity.

JaeYoung Han

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Since 2016, the National Institute for International Education has been supporting pre-service teachers to go abroad and do educational volunteer activities focusing on mathematics, science, and IT. Pre-service teachers are not accustomed to giving lessons yet, so they cannot teach foreign students alone in the local language. So they teach in a group of 3 to 4 members. Coteaching is the process by which many people prepare, implement, and evaluate classes together, and pre-service teachers get many opportunities for mutual learning through co-teaching during educational volunteer activities. While previous studies on co-teaching mainly deal with the coteacher's interaction in the cognitive domain, this study investigates the affective experiences of pre-service teachers in volunteer coteaching. The effects of coteaching were divided into positive and negative aspects by analyzing reports and evaluation records written by Chungbuk National University volunteers. Positive experiences of co-teaching include gratitude, mutual encouragement, sharing of confidence, learning passion for classes, exchanges of various teaching perspectives, and affection with peers and students. Negative experiences include dispersion of responsibility, sorry for not being able to help enough, worry (frustration) compared to one's own class, reflection on one's own shortcomings, and experiencing difficulty in teaching. The affective experiences of the overseas volunteers can be used as reference materials to communicate with each other in the future volunteer activities. (This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2018S1A5A2A01036487))

Poster Presentation : **EDU.P-422**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Case Study on Science Teachers’ Enactment of NOS Assessments : Focus on ‘Scientific Inquiries in the History’ of Science Inquiry Experiment

Haerheen Kim, Minhwan Kim, Taehee Noh*

Department of Chemistry Education, Seoul National University, Korea

In this study, we deeply investigated the cases of science teachers who enacted NOS assessments in Scientific Inquiry Experiment. Two science teachers working at high schools located in Seoul who taught and assessed NOS in Scientific Inquiry Experiment according to the 2015 revised curriculum participated in the study. We collected lesson and assessment materials and observed NOS lessons and assessments. We also conducted interviews. Based on the collected data, we analyzed processes of teachers’ enacting NOS assessments. The analyses of the results revealed that teachers constructed the assessments by themselves due to a lack of NOS assessment experience and related materials. They had difficulties in selecting appropriate assessment method and constructing assessment questions and criteria. Both teachers thought that it was difficult to assess the understanding of NOS because it is subjective view of individual students. Therefore, they had difficulties in setting detailed assessment criteria, which also led to difficulties in the overall assessment process. There was a difference in the reflective level of the assessments by the two teachers. In the reflective activities of low level, the assessments were not properly enacted because it was difficult to infer students’ understanding. Orientations toward teaching NOS influenced the perception of NOS assessment and overall lessons, resulting in a difference in NOS assessments. Finally, the absolute evaluation of Scientific Inquiry Experiments also affected teachers’ NOS assessments. Based on the above results, implications for effective NOS assessments in schools are discussed. (This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea(NRF-2021S1A5A2A01061452))

Poster Presentation : **EDU.P-423**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Recognition of observation and communication in inquiry class for science gifted students

Wonho Choi*, Hyowon Kim[1]

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

In this study, we analyzed the problem recognition, hypothesis setting, variable control, and class awareness of middle school science gifted students who participated in inquiry classes emphasizing observation and communication. For the problem recognition ability of the students, there were 4 types for the criterion of 'do you select a question that can be explored', and 3 types for the criterion of 'do you state the problem so that the independent and dependent variables are clearly revealed'. For the ability to set hypotheses of the students, there were 6 types for the criteria of 'thought process to explain the relationship between variables'. Also, for the variable control ability, there were 3 types for the criterion of 'level of operating variable', 2 types for the criterion of 'level of control variable', and 3 types for criterion of 'level of dependent variable'. After the class, a class awareness test was conducted to see how observation and communication activities had an impact on the progress of inquiry activities. And based on the students' research reports and class awareness results, we tried to find implications for science gifted students in middle school.

Poster Presentation : **EDU.P-424**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A survey of students' perceptions of STS in classes for high school students applying SWH(Science Writing Heuristic)

Wonho Choi*, **Haneul Lee**[1]

Department of Chemistry Education, Sunchon National University, Korea
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This study investigated the perception of STS and the class in the inquiry class to which SWH(Science Writing Heuristic) was applied to high school students. Classes were held for 4 days, 5 hours a day, and students explored the properties of liquids. On the first day, research problem was provided, and after the second day, students set up research problem based on previous experiment results and proceeded with exploration. Students came to recognize that there is an interaction between science and technology through class. The reasons for this included the everyday idea that science interacts with technology, the experience of improving tools to solve problems, the idea that new experimental results can be obtained with the help of technology, and the experience of applying science to real life.

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Poster Presentation : **EDU.P-425**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An Analysis of Science Teachers' NOS Lessons : In the Context of ‘Scientific Inquiries in History’ of Science Inquiry Experiment

Minhwan Kim, Taehee Noh*

Department of Chemistry Education, Seoul National University, Korea

In this study, science teachers’ NOS lessons were observed and the characteristics of the lessons were analyzed. Three science teachers who taught NOS in the ‘Science Inquiry Experiment’ developed under the 2015 revised curriculum participated in the study. Their NOS lessons were observed and interviews were conducted before and after lessons. The collected data were analyzed using analytical induction and constant comparative method. The analyses of the result revealed the teachers' naive views on NOS were also revealed during the lessons. There were some cases where they showed naive views during the lessons even if they showed informed views in the interviews. Although the domains of NOS taught by them were diverse, all of them taught ‘tentativeness’ and considered this an important goal. They tended to teach NOS with content related with their major, and teaching NOS was found to be deeply related to their major. In the activity where students learn NOS by inferring the unknown object, teachers disclosed the unknown object, which is unlike the rule of the activity. They thought that could help students’ learning. At last, although they emphasized teaching NOS, they either did not assess NOS or assessed NOS in a limited way. Based on the results, some directions for teacher education and follow-up study are suggested.

Poster Presentation : **EDU.P-426**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An Analysis of Pre-service Science Teachers’ NOS-PCK : In the Context of ‘Scientific Inquiries in History’ of Science Inquiry Experiment

Minhwan Kim, Haerheen Kim, Taehee Noh*

Department of Chemistry Education, Seoul National University, Korea

In this study, we investigated pre-service science teachers’ NOS-PCK by analyzing their NOS lesson planning and demonstration. Four pre-service science teachers participated in the study. They planned and demonstrated NOS lessons in the context of ‘Science Inquiry Experiment’ developed under the 2015 Revised National Curriculum. Their lessons were observed. All of the teaching-learning materials were collected, and semi-structured interviews were also conducted. The analyses of the result revealed that pre-service teachers mainly referred to the curriculum and textbooks when selecting the NOS learning objectives. However, they felt difficult because the curriculum and textbooks did not clearly present the NOS to be dealt. Although all of them took explicit approaches, there were not many open and divergent reflective approaches. In addition, they expected that high school students would consider scientific knowledge absolute and would have negative perceptions of NOS lessons. They rarely assessed students’ NOS learning, and were reluctant to assess. Finally, most of them had a negative perception that learning NOS was not necessary for all students. On the bases of the results, educational implications for improving the expertise of pre-service science teachers in NOS lessons were discussed.

Poster Presentation : **EDU.P-427**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Analyzing the Context-based Characteristics of Pre-service Science Teachers' Reflection of Questions

Sunghoon Kim, Yousun Jeon[1], Hunsik Kang[2], Taehee Noh[1,*]

Seoul National University, Korea
[1]*Department of Chemistry Education, Seoul National University, Korea*
[2]*Elementary Gifted Education, Seoul National University of Education, Korea*

The purpose of this study is to develop the workshop to improve teachers' questions considering the context of discourse. Four pre-service science teachers in the fourth grade participated in the study. Pre-service science teachers participated in the workshop. The characteristics of their reflection on the question considering the context of discourse were analyzed. Pre-service science teachers considered the types of questions they learned in the workshop during the reflection. But the affective domains of students were rarely considered. Whether the students respond was considered as an important factor of reflection. The questions were evaluated based on the frequencies. A single question without context was reflected on. Various PCK elements were not considered comprehensively. Based on the results, the practical implications to develop a program for improving teacher expertise related to the questions considering the context of discourse were discussed.

Poster Presentation : **EDU.P-428**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An Analysis of PCK Components in Elementary Science Teacher's Guides for 3rd~4th Grade developed in 2015 Revised National Curriculum

Nayoon Song, Taehee Noh[1,*]

Center for Educational Research, Seoul National University, Korea

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

We analyzed the PCK components in the material units of the 3rd to 4th grade of the elementary school teacher's guides developed under the 2015 revised national curriculum. The result revealed that the PCK components were presented in a relatively balanced manner compared to the teacher's guides in middle school. Knowledge of subject matter accounted for the highest proportion, and knowledge of instructional strategies in science was a higher proportion than knowledge of science curriculum. Knowledge of assessment in science showed the greatest deviation among publishers, and knowledge of students was the lowest in most publishers. By sub-components, the proportion of experiments and inquiries was higher than that of concepts and theories. The ratio of horizontal articulation was lower than that of vertical articulation or lesson objectives, and lesson objectives were presented in various ways such as science core competencies and achievement standards. As questioning was emphasized, teaching strategies and questioning appeared at a similar rate. Motivation and interest, misconceptions were linked to teaching strategies and questioning. In some cases, assessment items and assessment criteria were presented for each level, and various PCK components were linked around these two components. Components with relatively large differences among publishers were supplementary or in-depth concepts, inquiry in textbooks, instruction sequence and method, subject-specific strategies, and assessment items. Based on the results, implications for the development of teacher's guides were discussed.

Poster Presentation : **EDU.P-429**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Context-based Analysis of Pre-service Science Teachers' Questions in Teaching Practices

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

In this study, pre-service chemistry teachers' questions in their teaching practices were analyzed considering the context of discourse. Five pre-service teachers participated in the study. Their questions were analyzed by considering various data including class videos, interviews, and teaching-learning materials. Their questions were classified into relevant question, affective question, dead-end question, rhetorical question, and structuring question. Each question was also classified into appropriate question and convenient question by the aspect of proper responses of students. The analyses of the results indicate the differences in the frequencies of several types of questions depending on the content of the lessons. After using convenient questions, pre-service teachers proceeded to prepared classes as they rather than prompted students' responses. The affective questions were rarely used. The dead-end questions were found to be used for promoting interaction with students. The rhetorical questions were used for various purposes such as arousing students' attention or promoting their thinking. Practical implications were discussed based on the results.

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Poster Presentation : **EDU.P-430**
Chemistry Education
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The Form, Presentation, and Interactivity of External Representations in Elementary Science Digital Textbooks: Focused on Matter Units

Haerheen Kim, KiDoug Shin, Taehee Noh, Minhwan Kim[*]

Department of Chemistry Education, Seoul National University, Korea

In this study, we analyzed the form, presentation, and interactivity of external representations presented in matter units of the elementary school science digital textbooks developed under the 2015 Revised National Curriculum. The analytic framework of the previous study was modified and supplemented. We analyzed the matter units in the 3rd-6th grade science digital textbooks by dividing them into ‘body texts’ and ‘inquiries’ area. The analyses of the results revealed that visual-verbal representations and visual-nonverbal representations were presented the most. On the other hand, audial-nonverbal representations were presented at a high frequency only in the body texts, and audial-verbal representations were presented at a low frequency in both the body texts and the inquiries. In terms of the presentation, when verbal representations and visual-nonverbal representations appeared together, visual-verbal representations and visual-nonverbal representations were mainly presented together. In some of the cases where visual-verbal representations, audial-verbal representations, and visual-nonverbal representations were presented together, information on visual-verbal representations and audial-verbal representations was presented redundantly. Audial-nonverbal representations unrelated to contents were presented along with other external representations, and the frequency was particularly high in the body texts. In terms of the contiguity, none of visual-verbal representations and visual-nonverbal representations were presented on different pages, and none of audial-verbal representations were presented asynchronously with visual-nonverbal representations. In terms of the interactivity, explanatory feedback and low-level manipulations were mainly presented. Based on the results, implications to improve digital textbooks are discussed from the perspective of multiple representation-based learning.

Poster Presentation : **EDU.P-431**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An Analysis of Pre-service Science Teachers' Reflection of Questions in Terms of Productive Reflection

Sunghoon Kim, Yousun Jeon[1], Hunsik Kang[2], Taehee Noh[1,*]

Seoul National University, Korea
[1]*Department of Chemistry Education, Seoul National University, Korea*
[2]*Elementary Gifted Education, Seoul National University of Education, Korea*

In this study, we investigated pre-service teachers’ reflection of questions during science instruction in teaching practicum from the perspective of productive reflection. The productive reflection used in this analysis has four aspects of learners and learning, subject matter knowledge, instruction, and assessment. Five pre-service teachers participated in this study. They reflected on their questions with one class video by using think-aloud method. Semi-constructed interviews were also conducted. The analyses of the results reveal that the aspect of ‘instruction’ and the ‘learners and learning’ were frequently included in their reflections. ‘subject matter knowledge’ was often included in their reflections while ‘assessment’ was hardly included. The integrations of the two aspects appear most often, those of the three aspects appear only sometimes. However, four aspects appear very rarely. The integrations of ‘learners and learning’ and ‘instruction’ with the other aspects were most frequent, and the integrations of ‘content knowledge’ with the other aspects were often. However, the integration of ‘assessment’ was very few. There were more productive reflections from pre-service teachers who reflect on several questions in context than who reflected on questions one by one. In addition, they exhibited some difficulties in suggesting alternatives to improve their questions. They tried to modify the teaching method related to the questions rather than revise the form of the questions. Based on the results, practical implications to improve expertise related to the questions of pre-service teachers were discussed.

Poster Presentation : **EDU.P-432**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The effect of the chemistry experiments utilizing high tech equipment of science high school on the affective characteristics in science aspect of ordinary high school students

Jihun Park, Jeonghee Nam*, HongGyeong Park

Department of Chemical Education, Pusan National University, Korea

This research was conducted for understanding of ordinary high school students’ affective-characteristics change on the science, when they meet new environment for chemistry lesson with high-tech equipments brought from science high schools.And for this purpose, we have developed six new courses relying on high-tech apparatus such as UV-VIS spectrometer and NMR. Before and after all lessons were finished for those courses, we searched about students' opinion with pre- and post- test surveys on affective characteristics were conducted, followed by questionnaire-survey on program features and interviews. As a result, first, we did confirm the significant effect of those courses on ordinary high school students' affective characteristics. First of all, they could experience career aspirations which would be rarely talked in ordinary high schools — and that could happen due to experiences such as operating advanced analysis equipment, implementation of experimental activities, etc. But also various chemical experiences through professional activities have influenced a lot for perception on chemistry. Admittedly, for current education-scheme cycle, our suggestions can tell only for extracurricular programs. But certainly at least, it would tell a lot for future plans on educational policy, including compilation, subject operation and others getting involved with joint curriculum prospectively

Poster Presentation : **EDU.P-433**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Pre-service Chemistry Teachers' Beliefs Related to Teaching and Learning

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

The purpose of this study is to explore pre-service chemistry teachers' beliefs related to teaching and learning. The beliefs of 75 pre-service chemistry teachers were measured using a measuring tool for beliefs consist of the traditional approach (8 items) and the constructivist approach (5 items) developed by Woolley, Benjamin, & Woolley (2004). The Cronbach’s α of the measurement tool was .758 in the traditional approach and .745 in the constructivist approach. As a result of the study, the average of all questions for the traditional approach was 3.62, and the average of the constructivist approach was 3.93. The constructivist approach was slightly higher than the traditional approach, this difference was statistically significant (t=-3.352, p

<u>Mihyun Son</u>, Dae Hong Jeong[1,*]

Division of Natural Sciences, Seoul National University, Korea
[1]*Department of Chemical Education, Seoul National University, Korea*

Boiling point elevation phenomenon is a good concept that can draw students' interest in real life, but it appears as an equation with molality as an independent variable. Therefore, only some students who choose Chemistry II are learning based on formulas. The purpose of this study is to find the best experimental conditions to understand boiling point elevation through experiments and to find the possibility which is explaining the quantitative relationship of boiling point elevation by molarity or mole fraction, not molality. The study found that the quantitative relationship between molality and boiling

point elevation was described in all textbooks, and the linearity of boiling point elevation to 5 m concentration was confirmed, and the theoretical value was more approximated when it was a dilute solution of 2 m. The best experiment result was drawn in a graph showing that both molarity and mole fraction and theoretically, it was possible to explain boiling point elevation using them in dilute solution. The purpose of this study is to find ways for more students to understand and experiment with concepts useful in real life, such as boiling point elevation, which can be used in textbooks or curriculum improvement and optional subject classes.

Poster Presentation : **EDU.P-434**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Where is the freezing point of a supercooled aqueous solution of NaCl?

Dae Hong Jeong*, Myoung Joo Baek

Department of Chemical Education, Seoul National University, Korea

In this study, we measured the temperature change of 1m(molarity) of aqueous NaCl solution in nature using a waterproof temperature sensor(DS18B20) with a wireless Arduino board(esp8266). We recorded the sensor values in real-time using Thingspeak (http://thingspeak.com) and captured phase changes via video recording. The freezing-point depression in chemistry textbooks is commonly presented as theoretically converged experimental values. But Supercooling was observed in an aqueous solution of NaCl at temperatures below minus 10 degrees Celsius. External irritation can drastically change the state of liquids below freezing point. Laboratory and classroom measurements of freezing points have been hindered by this supercooling. This phenomenon, however, can also be explained by observing a change in state in conjunction with an exothermic reaction. Thermodynamic analyses such as enthalpy, entropy, and Gibbs free energy are also available. Our discussion focused on the freezing-point depression in solutions based on a theoretical review. To analyze the changes in the supercooled state, we also examined the case of temperature measurement in the natural.

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Poster Presentation : **EDU.P-435**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An Analysis on the Performance Assessment Plan in the ‘Chemistry I’ of the 2015 Revised Curriculum

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[1] *Division of Science Education, Kangwon National University, Korea*

The purpose of this study is to find out how the performance evaluation of 'Chemistry 1' in the 2015 science curriculum is being conducted. To this end, general high schools across the country were proportionally sampled based on basic education statistics, and science performance evaluation plans announced in school notices were collected and analyzed. The collected evaluation plans were classified based on the skill level of the evaluation criteria, subject of evaluation, type of performance evaluation, relevant unit and contents, etc. Based on the analyzed results, difficulties and problems of performance evaluation were discussed through 'Focus Group Interview'.

Poster Presentation : **EDU.P-436**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Empirical Investigation on 'Boiling Point Elevation

Mihyun Son, Dae Hong Jeong[1,*]

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Boiling point elevation phenomenon is a good concept that can draw students' interest in real life, but it appears as an equation with molality as an independent variable. Therefore, only some students who choose Chemistry II are learning based on formulas. The purpose of this study is to find the best experimental conditions to understand boiling point elevation through experiments and to find the possibility which is explaining the quantitative relationship of boiling point elevation by molarity or mole fraction, not molality. The study found that the quantitative relationship between molality and boiling point elevation was described in all textbooks, and the linearity of boiling point elevation to 5 m concentration was confirmed, and the theoretical value was more approximated when it was a dilute solution of 2 m. The best experiment result was drawn in a graph showing that both molarity and mole fraction and theoretically, it was possible to explain boiling point elevation using them in dilute solution. The purpose of this study is to find ways for more students to understand and experiment with concepts useful in real life, such as boiling point elevation, which can be used in textbooks or curriculum improvement and optional subject classes.

Poster Presentation : **EDU.P-437**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

The role of laboratory instruction in science education: From the perspective of Liebig in the 19th century

Seonyeong Mun, Gyeong-Geon Lee[1], Hun-gi Hong[2,*]

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Laboratory instruction has been an important part of modern science education. However, there are many different arguments about its purpose and it has been suggested that the shape of laboratory instruction can differ according to what each instructor wants to provide students with. There have been also calls for a synthetic framework for laboratory instruction to improve it. Justus von Liebig (1803-1873), a renowned 19th-century scientist, is regarded not only as a scientist who made intellectual advances in various fields such as organic chemistry, medicine, pharmacy, physiology, and agriculture, but also as a person who made a mark on chemistry education by systematizing German university laboratories. In the process of raising the status of chemistry in Germany, Liebig emphasized the necessity and importance of chemistry education and experimentation. In this respect, examining the purpose of laboratory instruction from Liebig's perspective can provide an answer for the purpose of laboratory instruction. In this study, we examine Liebig's thoughts on the purpose of the laboratory instruction and his activities in which these appeared. Specifically, his research experiences in Germany and France that influenced Liebig's thoughts were examined, followed by an exploration of the meaning and purpose of experimentation from his perspective. The tools and laboratory instruction in which Liebig's ideas were reflected were then scrutinized, along with the need for public chemistry education as suggested by Liebig. Finally, based on these, the implications for laboratory instruction in science education were discussed.

Poster Presentation : **EDU.P-438**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Development of college classes to improve pre-primary teachers' ability to organize arguments on Socio-Scientific Issues (1)

Young Tae Kong

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The purpose of this study is to develop a university curriculum to improve the ability of pre-elementary school teachers to organize arguments on Socio-Scientific Issues.In this study, a class module [1] based on a topic related to the construction of a nuclear power plant, which is of high social interest in Korea, was developed. And the developed class module was applied through non-face-to-face classes from March to May 2020 for sophomores at the university of education.[1] Kusumi A. (2017). The first nuclear power plant guidebook. Tokyo: SOSEI publisher.This research was partially supported by the National Research Foundation of Korea (2016R1D1A1B02008712).

Poster Presentation : **EDU.P-439**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Analyzing the effectiveness of chemistry teaching and learning programs based on metacognitive learning strategies using AR/VR contents and surveying perceptions

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[1]*Division of Science Education (Chemistry), Jeonbuk National University, Korea*

The purpose of this study is to investigate the effect and perception of chemistry teaching and learning programs using realistic contents on pre-service teachers' creative thinking competencies and core competencies of science subjects. In particular, it was intended to further improve the effectiveness of the program by introducing a strategy to strengthen metacognition. The participants were classified into the experimental class, which is applied with the newly developed chemistry teaching and learning program, and the traditional class, which is applied with a general program that does not include realistic contents and metacognitive strategies. Self-assessment questionnaires were conducted before and after the application of the program to both groups to measure the degree of change in metacognitive competency, creative thinking competency, and core competency in science subjects. As a result of the study, the metacognitive competency, creative thinking competency, and some of the science and core competencies of the experimental group, which were applied with programs including realistic content and metacognitive strategies, were significantly improved. On the other hand, there was no difference before and after the competency of the traditional class to which the general program was applied. As a result of the perception survey, the experimental group showed a significant difference in the question that it would help improve students' interest and participation, metacognitive competency, and creative thinking competency when classes were conducted using the experienced program. As a result of analyzing the free response, it was positively recognized that the experimental class to which the developed program was applied was helpful to interest and participation because it could stimulate audio-visual, and that student participation was the center. However, it was negatively recognized that the application had frequent errors and the degree of freedom was low in the process. Through the results, implications for the development of a learning model and program combining metacognitive learning strategies with the

use of realistic content, error correction of applications, and development of realistic content with a high degree of freedom were obtained.

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Poster Presentation : **EDU.P-440**
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Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A Study on the Change in Science Grades and the Influence of Science Grades by Level according to Non-face-to-face and Face-to-face Teaching-Learning

MInJu Koo, Jong Keun Park*

Department of Chemical Education, Gyeongsang National University, Korea

We compared and analyzed the changes in students' science grades and their effects on science grades by level (upper, middle, and lower) according to non-face-to-face and face-to-face teaching-learning. 66 students from A Middle School in Gyeongsangnam-do were selected for the study. As a result of analyzing the change in science grades according to the teaching-learning type, the average score of science grades by non-face-to-face teaching-learning was lower than the corresponding score of science grades of face-to-face teaching-learning. As a result of comparing the level of understanding of learning content according to the evaluation type (paper-written, study-paper) in non-face-to-face and face-to-face teaching-learning, the average scores of science grades by paper-written and study-paper evaluations in non-face-to-face teaching-learning were significantly low. In addition, as a result of comparing the effect on science grades by level according to the teaching-learning type, the average score of science grades of lower-ranked students in non-face-to-face teaching-learning was relatively low.

Poster Presentation : **EDU.P-441**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effectiveness Analysis of Online Mathematics and Science Virtual Laboratory Programs: For underprivileged high school students

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In this study, online mathematics and science virtual laboratory contents were developed and applied to underprivileged high school students. Through this, the purpose is to verify the effectiveness of applying laboratory contents for online mathematics and science in science classes of high school students. In particular, we tried to verify the effectiveness of the program through changes in students' affective attitudes in the learning process. The program used 'molecular model virtual laboratory' and 'acid and base neutralization proper virtual laboratory' contents developed by the Korea Institute of Science and Technology Information (KISTI). A virtual experiment manual was developed and teacher training was conducted so that field teachers could conduct classes. Participants are high school students in the laboratory class who are applied to the newly developed online math and science virtual laboratories in class. A self-evaluation questionnaire was conducted before and after the application of the program to measure the degree of change in the science positive experience index. The data were analyzed by descriptive statistics and corresponding sample t-verification using SPSS 27. As a result of the study, it was found that students who were applied to the online math and science impersonation lab program significantly increased their science learning emotions, science-related self-concept, science learning motivation, science career abandonment, and science-related attitudes after the program was applied. Meanwhile, as a result of analyzing the change in science positive experience indicators according to the sex of the students in the laboratory class who were applied to the online math and science virtual lab program, the difference between pre-test and post-test of female students was significant at a higher significance level than male students. Based on these results, it is expected that the gap in learners' academic background according to regional and school conditions and educational environments can be bridged by developing online mathematics and science virtual laboratory learning models and programs.

In addition, through the integration with convergence education, implications for diversification of content topics and contents, and edutech teaching and learning methods were obtained.

Poster Presentation : **EDU.P-442**

Chemistry Education

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigating the Educational Effects of Using Electronic Inquiry Notes in Student Inquiry Activities.

Namsoo Lee, Byeong-Seon Kim*

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This study investigates the educational effects of using Electronic Inquiry Notes(EIN) when students perform inquiry activities, in order to support the enhancement of digital literacy, future competency, and process-oriented evaluation, which are promoted in the 2022 revised curriculum. The study developed an electronic inquiry note program to provide students with assistance in knowledge information processing and report writing during their learning process, and to enable teachers to conduct process-oriented evaluation through open inquiry reports. The study analyzed students' satisfaction, achievement, and learning difficulties, and investigates the impact of introducing electronic inquiry notes on student learning.

Poster Presentation : **EDU.P-443**
Chemistry Education
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Analysis of the Cognition Level of the Nature of the Model Shown in the Modeling Practices Using Technology of Pre-service Chemistry Teachers

Najin Jeong, Seounghey Paik*

Department of Chemical Education, Korea National University of Education, Korea

Model is a key component of the scientific inquiry process. The Next Generation Science Standards emphasize developing student's ability to create models based on evidence as an important goal of science education. Due to this influence, the development and use of models are emphasized in the 2015 revised curriculum and the 2022 revised curriculum of science education in Korea. In order to properly develop and use models in science classes, teachers must have a clear cognition of the nature of models. In this study, cognition level of the nature of the model was analyzed which was shown in pre-service chemistry teachers' modeling practices using technology. As a result, it was found that pre-service chemistry teachers had a high cognition level in the representational aspect of the nature of the model, but they had a low cognition level in the explanatory aspect. Therefore, it is suggested that the education of pre-service teachers is necessary to properly recognize the nature of the model in the explanatory aspect.

Poster Presentation : **ENVR.P-444**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A study of nitrogen enriched porous carbons for carbon dioxide adsorption

Jong-Hoon Lee, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this study, porous carbons with high porosity were synthesized by chitosan which known as abundant polysaccharide. The precursors were carbonized at 900℃, 1 hr, and N_2 flow conditions using chitosan as carbon precursor. After carbonized, porous carbons were synthesized by chemical activation. The effect on quantity of activation reagents was investigated by experience of carbon precursor/chemical reagent mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N_2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **ENVR.P-445**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation and characterization of microporous carbons for high-pressure methane adsorption

Jong-Hoon Lee, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Using porous adsorbent at relative low pressure and room temperature is one of promising technique for natural gas storage. In this study, activated carbons (AC) with high microporosity were synthesized by nitrogen-enriched precursors. The precursors were carbonized at 900℃, 1 hr, and N_2 flow conditions. After carbonized, AC was synthesized by chemical activation. The effect of quantity of activation reagents was investigated by experience of AC/chemical reagent mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N_2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The microporosities of samples were evaluated using non-local density functional theory (NLDFT). Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **ENVR.P-446**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile synthesis of highly porous carbon nanotube aerogels for gas adsorbents

Jong-Hoon Lee, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Carbon nanotube-based aerogels attract attention due to the high surface area and porosity. In this study, carbon nanotube aerogels were synthesized by carbon nanotubes and chitosan. Chitosan and CNT was dissolved in 1M HCl solution. The Chitosan/CNT mixture were freeze dry for preparing aerogels. Aerogels were carbonized at 200℃, 1 hr, and N_2 flow conditions. After carbonized, prepared samples were washed using water and ethanol until neutralization. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N_2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The pore size distributions were investigated using non-local density functional theory (NLDFT).

Poster Presentation : **ENVR.P-447**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

A study of photoreduction properties of Cr(VI) in electrospun composite nanofibers: analysis of the effect of multi-walled carbon nanotube content

Su-Bin Kim, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Titanium dioxide ($TiOH_2$), the most widely used photocatalyst, has excellent stability, low price, and strong oxidizing power, but its efficacy in visible light is limited. To address these limitations and improve the photocatalytic efficiency to control the range, a composite photocatalyst was fabricated by incorporating multi-walled carbon nanotubes (MWCNTs) into pristine $TiOH_2$, which was synthesized via electrospinning using poly(vinylpyrrolidone). Enhancement of the specific surface area promoted by the presence of multi-walled carbon nanotubes (MWCNTs) increases photocatalytically active sites Band gap control and prevention of electron-hole recombination Photoreduction properties MWCNTs/$TiOH_2$ composite nanofibers were developed in aqueous solution under sunlight. The decomposition efficiency of chromium (VI) was investigated and quantified. As a result, it was found that the decomposition rate of Cr (VI) increased as the content of MWCNTs increased. In conclusion, the incorporation of MWCNTs is related to adsorption of harmful substances, control of the band gap of $TiOH_2$, it improves the photoreduction efficiency due to the nanofiber structure produced by electrospinning.

Poster Presentation : **ENVR.P-448**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Preparation of MWCNTs/TiO_2/WO_3/Multi-walled carbon nanotube composites for photoreduction of chromium (VI) under visible light irradiation

Su-Bin Kim, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

The unique properties of nanomaterials have made them highly desirable in the field of photocatalysis. Specifically, their larger absorption cross-section extends the absorption range of visible light. In this study, a photocatalyst was prepared by incorporating WO_3 into electrospun TiO_2/MWCNTs through hydrothermal synthesis. The increased specific surface area due to the presence of MWCNTs enhances the active sites of the photocatalyst and improves its ability to adsorb harmful substances. The photoreduction properties were analyzed by controlling the bandgap in an aqueous solution under visible light, with the addition of WO_3. Results showed that the decomposition rate of Cr(VI) in visible light increased as the amount of WO_3 increased. In conclusion, the incorporation of WO_3 into TiO_2 leads to bandgap control and improved photoreduction efficiency due to the nanofiber structure created by electrospinning. However, an excessive amount of WO_3 may promote the recombination of electron-hole pairs.

Poster Presentation : **ENVR.P-449**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Synthesis of waste cigarette butts-derived activated carbons for hydrogen uptakes

Choong-Hee Kim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

The solid materials for hydrogen adsorption including carbonaceous materials, metal-organic frameworks, and zeolites have been extensively investigated to increase their specific surface area (SSA) and porosity to maximize the amount of hydrogen uptake onto the materials. Most of the effort in this field has focused on developing the porosity of the materials. However, the hydrogen uptake of the materials depends not only on the SSA but also on its surface characteristics, if not more so, which effect on the interaction between adsorbent (storage materials) and adsorbate (hydrogen molecules). To understand these factors in detail, we undertook an investigation to study the hydrogen uptake, the surface functionality and textural property of oxygen-rich porous carbons prepared by carbonization and subsequent activation using cigarette butts as a precursor. In this work, we also suggested the efficiency factor of the pore size of the materials for hydrogen adsorption.

Poster Presentation : **ENVR.P-450**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Effect of silica elimination process to highly micropores on pine cone-derived activated carbons for carbon dioxide capture

Choong-Hee Kim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Biomass-based activated carbons (ACs) are widely used as CO_2 capturing materials. The silica elimination process (SE) has rarely been studied for developing the porosity of ACs. Here, we prepared pre-carbonized pine cones (CPC) as a starting material to investigate optimizing the micropores of ACs according to the preparation sequence. One was prepared by chemical activation (CA) and the subsequent SE (CPC-CA-SE/ACs) and the other was carried out the SE before CA (CPC-SE-CA/ACs). From the results, we found that the preparation sequence had a strong effect on the textural properties of the resultant of biomass-based ACs and their CO_2 capture performance.

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Poster Presentation : **ENVR.P-451**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Facile synthesis of Ti_2C_3 MXene decorated Bi_2O_3 photocatalyst

Jishu Rawal, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Ti_2C_3 MXene assisted Bi_2O_3 photocatalysts were synthesized via two processes i.e., hydrothermal process and calcination process. Two methods of preparation were employed to calibrate and precisely operate the synthesis method of photocatalyst for the enhanced photodegradation of organic pollutant and antibiotics. Different mass loading of MXene was used as a sensitizer to rationalize the nanocomposite composition. The morphology, crystal structure, optical spectroscopy, thermal stability, surface properties, visible light photocatalytic activity, and photoelectrochemical activity of as-prepared photocatalysts were systematically analyzed and discussed. Results show that Ti_3C_2 nanosheets play an important role in widening the absorption region of $Bi2O_3$ nanoparticles. However, the stable interface of Ti_3C_2/Bi_2O_3 accelerates the charge separation and transfer of electrons. The scavenger experiment also specifies the role of active species in photodegradation process. Thus, obtained Ti_3C_2/Bi_2O_3 photocatalyst attributes to the improved antibiotics and pollutant degradation.

131st General Meeting of the Korean Chemical Society
April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ENVR.P-452**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

One-pot synthesis of N, S-doped carbon dots/CdS heterostructures for improved photocatalytic degradation

Jishu Rawal, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Novel N, S-doped carbon dots/CdS nanocomposites were fabricated by simple one-pot synthesis method with different loads of N, S-doped carbon dots (NCDs). CDs were used as photosensitizer on the surface of CdS nanoparticles for the rapid electron-hole pair transport on the excitation of visible light. The NCDs/CdS nanocomposites were used to degrade organic pollutant dye and antibiotics through photocatalysis process. The results were comparatively scrutinized to study the role of NCDs on CdS nanoparticles. The as-prepared NCDs/CDS samples has achieved high photodegradation efficiency due to stable heterojunction formation and proper bang gap alignment, i.e., also beneficial for the improvement of visible light absorption, high carrier charge transfer, and strong redox ability. Moreover, the mechanisms of photodegradation over as-prepared heterojunctions were elucidated.

Poster Presentation : **ENVR.P-453**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Visible-light driven superior photocatalytic performance of Ti_2C_3 MXene/CdS quantum dots

Jishu Rawal, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Ti_2C_3 MXene/CdS quantum dots were synthesized via a hydrothermal method. The products were characterized by X-ray powder diffraction, scanning electron microscopy, transmission electron microscopy, X-ray photoelectron spectroscopy, Fourier-transform infrared spectroscopy, thermogravimetric analysis, gas adsorption analyzer, UV–vis absorption spectroscopy, and Ivium electrochemical analyzer. The formation mechanism for the Ti_2C_3 MXene/CdS quantum dots was discussed. The prepared Ti_2C_3 MXene/CdS quantum dots showed the superior photocatalytic activity for the degradation of organic dye under visible light irradiation and were found to be highly efficient for organic pollutants and antibiotics removal. Moreover, this catalyst showed improved stability up to four recycles. The unique structure may favor the harvesting of exciting light due to multiple scattering within the interior space, and the incorporation of Ti_2C_3 MXene also facilitate the rapid generation of electrons and holes pairs and inhibit their recombination rate by acting as a temporary trapping sites of photoinduced electrons.

Poster Presentation : **ENVR.P-454**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

An easily scalable, durable, and highly efficient three dimensional solar evaporator inspired by a rice paddy field

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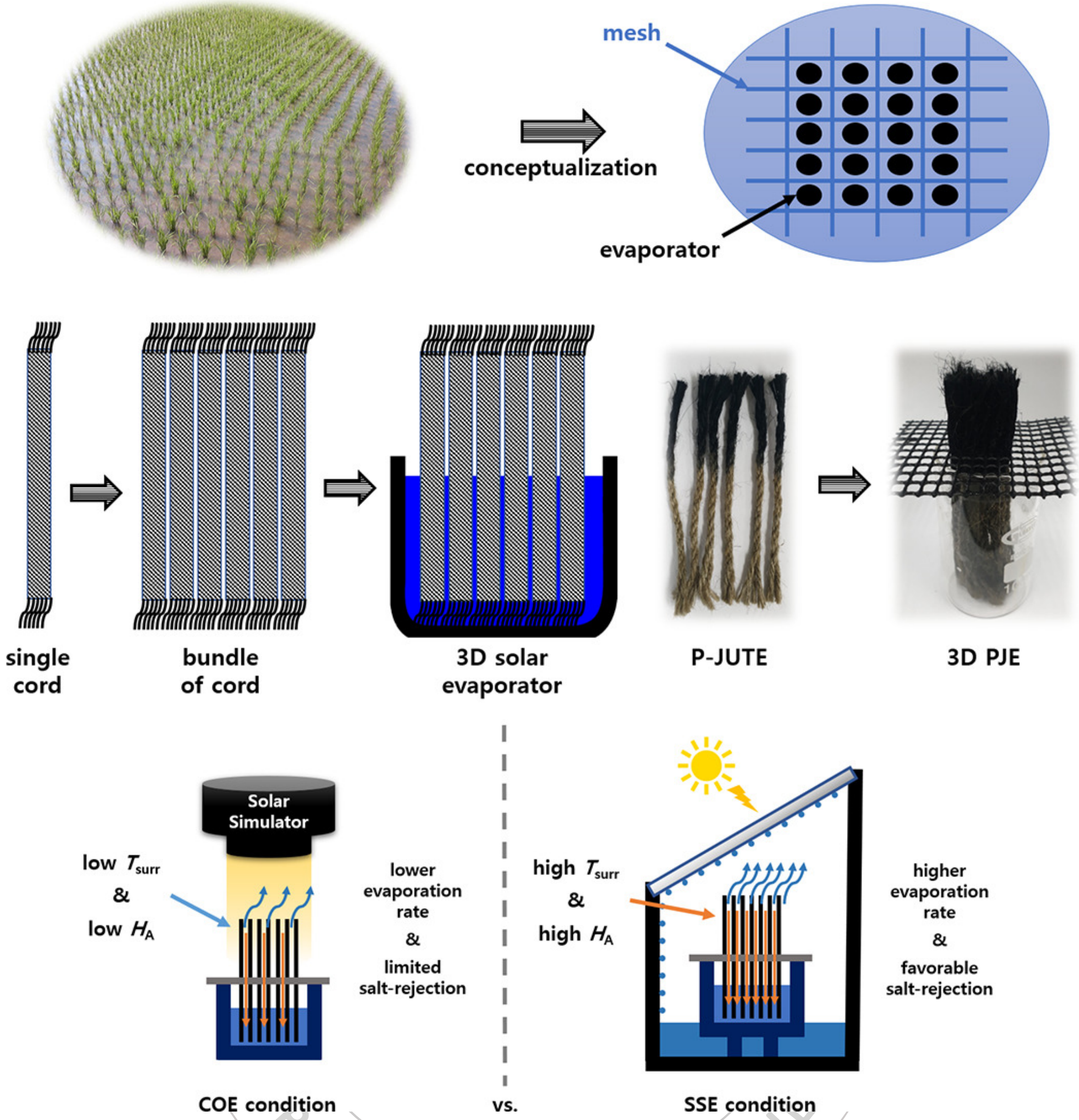
Interfacial solar evaporation is a crucial solution to address the growing issue of fresh water shortage. Despite advancements in solar evaporation systems, limitations such as scalability, ease of fabrication, cost, and efficiency still persist. This study presents a cost-effective, scalable, and efficient solution through interfacial solar evaporation using a 3D system inspired by a rice paddy field. Composed of vertically aligned and lattice-arrayed Polypyrrole(PPy) decorated 1D jute cords, the system exhibits high evaporation performance during a long-term simulated seawater evaporation experiment due to their good salt-rejecting capability. This result arises from the combined effects of the phtothermal performance of PPy and the vigorous side-surface evaporation accelerated by the acquisition of additional heat from the surroundings. The daily evaporation performance in a solar still field test was 33.24 kgm-2day-1 due to favorable temperature and humidity conditions. The results of this study emphasize the importance of sustainable solutions for fresh water production and shows the potential of the new 3D solar evaporation system as a promising solution.


mesh
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P-JUTE
3D PJE
Solar Simulator
low T_{surr} & low H_A
lower evaporation rate & limited salt-rejection
high T_{surr} & high H_A
higher evaporation rate & favorable salt-rejection
COE condition
vs.
SSE condition

Poster Presentation : **ENVR.P-455**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Bicontinuous SiO_2-Cu_xO_y-TiO_2 heterostructure prepared from Nanoporous Hybrid Fim (NHF) for Photocatalytic Applications

Kyeong Eun Yeo, Ji-Woong Park[1,*]

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TiO_2-supported catalyst has been in significant interest due to superior catalytic performance resulting from strong metal-support interaction (SMSI). However, the synthetic difficulty of porous TiO_2 structure with high surface area and the insufficient stability of catalyst supported on TiO_2 still impede extensive catalytic applications in many areas. In this context, bicontinuous SiO_2-Cu_xO_y-TiO_2 heterostructure was prepared from nanoporous hybrid film (NHF) as a template. The high chemical and thermal stability of NHF enable to produce highly crystalline bicontinuous structure with high surface area. In addition, the core-shell-like bicontinuous urea/organosilica network directly provides porous silica-coated Cu_xO_y-TiO_2 structure by sequent impregnation of metal and metal oxide precursors and pyrolysis without post-deposition of silica layer. The porous silica coating layer not only enhances catalytic stability of the copper compound during catalytic reaction, but also leads to unique electronic structure at the interface compared to none-coated Cu_xO_y-TiO_2 structure. Furthermore, electronic structure of catalyst can be easily modified by changing impregnation sequence of metal and metal oxide precursors. Such different electronic structures at the interface greatly influence electron density and charge transfer rate between copper catalyst and support, resulting in different catalytic activity and selectivity in photocatalysis. Here, we investigate how the structure and electronic structure of the catalyst heterostructure at the interface affect catalytic stability and activity in photocatalytic synthesis of chemical compounds.

Poster Presentation : **ENVR.P-456**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Characterization of Catalytic Removal of Aqueous Hg(II) on the Surface of Bimetallic ZIFs

Meiirzhan Nurmyrza, Woojin Lee*

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Mercury is a toxic chemical that can cause adverse human health effects, such as neurological and renal disturbances. It has been promulgated as one of the ‘ten leading chemicals of major public health concerns’ by the World Health Organization. Consequently, its maximum allowable concentration in drinking water was set at 1 μg/L. The consecutive anthropogenic emissions of this chemical to water bodies are causing severe environmental problems. Recent studies have shown the potential of reductive metallic catalysts for effectively removing aqueous Hg. Metallic catalysts supported by zeolite imidazolate frameworks (ZIFs) have been reported as an efficient adsorbent of vapor elemental Hg(0) via chemo- and physisorption. In this study, the ZIF-derived bi-metallic catalysts have been synthesized, characterized, and assessed for efficient aqueous Hg(II) removal. The batch kinetic tests have been conducted to characterize the catalytic Hg(II) reduction/removal on the surface of the ZIF-derived bi-metallic catalysts, including the Ru/ZIF-67, In/ZIF-67, Pt/ZIF-67, Ru-Co/NC, In-Co/NC, and Pt-Co/NC. The high Hg(II) removal (> 85%) has been achieved by Ru/ZIF-67 in 60 min and 15% of adsorbed Hg portion has been recovered on the catalyst surface. The aqueous Hg(II) could be effectively removed through the catalytic reduction and sorption mechanisms.

Poster Presentation : **ENVR.P-457**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Catalytic Removal of Aqueous Hg(II) on the Surface of Sn-Pd Bimetallic Catalyst Supported by Nano-Crystalline ZSM-5

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Mercury (Hg) is recognized to be among the most toxic heavy metals in existence that can easily damage human nervous and immune systems and disrupt the functioning of the major organs. 200 mg of methylmercury was estimated to be a lethal dose for a human. The US EPA set 10 ppb of Hg for the wastewater discharge limit, while the drinking water maximum contaminant level for Hg was done at 1 ppb. Current studies have been focusing on reductive metallic catalyst technologies to solve Hg contaminations in aquatic systems effectively and selectively. We synthesized the nanostructured crystalline zeolite (ZSM-5) through the hydrothermal synthesis method at 100 °C for 3 hours in a Teflon-coated autoclave. The bimetallic catalysts were prepared by impregnating the nano-porous ZSM-5 with Sn and Pd metals. The resultant reduced bimetallic 1%Sn-1.6%Pd-ZSM-5 catalyst was assessed for the catalytic reduction/removal of aqueous Hg(II) on its surface through batch kinetic tests. The synthesized bimetallic catalyst showed enhanced Hg(II) removals (> 85%) in 30 min with 25% of Hg(0) conversion in an aqueous solution, confirming the catalytic reduction and sorption mechanisms on the catalytic surface.

Poster Presentation : **ENVR.P-458**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photoelectrochemical wastewater treatment and hydrogen production from saline water desalination.

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The sunlight driven photoelectrochemical desalination cell is a novel system to obtain fresh water from wastewater and saline water. The photoelectrochemical cell consists of anode, desalination and cathode cells, each cells separated by ion-exchange membrane. Upon sunlight irradiation, a hydrogen treated TiO2 nanods (H-TNR) as a photo-anode generate electron hole pair and create electrical field in cell and then Chloride(Cl) and Sodium(Na) ions in saline water are desalted in desalination cell to anode and cathode cells through anion and cation exchange membranes. Desalted Cl ions are oxidized by photoanode to reactive chlorine species (RCS), that treatment wastewater in anode cell. Desalted Na ions increased the concentration of catholyte, improving the production of hydrogen in cathode cell. On the basis, stacked photoelectrochemical desalination cells were developed to enhance the desalination rate and energy efficiency in the present study. The specific energy consumption (SEC) of desalination cell numbers were investigated. Results showed that the SEC is decreased. Because an Ion transfer efficiency to increase. The SEC of 5 stack cell is 1.14 kWh cubic meter at 50% desalination of 10gL-1 NaCl saline water. Instead of Pt, Ni3S2-MoS2/Ni foam cathode continuously produced molecular of hydrogen at a faradaic efficiency of ~ 80%. AcknowledgmentThis research was supported by Basic Science Research Program through the NationalResearch Foundation of Korea(NRF) funded by the Ministry of Education(2022R1C1C201171211)Keywords: Photoelectrocatalyst, Desalination, Hydrogen production, Water treatment

Poster Presentation : **ENVR.P-459**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Enhancing the Electrochemical CO_2 Reduction Performance of Ag-Cu Electrodes through interface engineering by Electrodeposition.

Seon Young Hwang, Juyoung Maeng, Seo Young Yang, Goeun Park, Choong Kyun Rhee[1], Youngku Sohn[*]

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

Electrochemical CO_2 reduction has the potential to significantly reduce greenhouse gas emissions and mitigate climate change by converting CO_2 generated in various industrial processes and transportation into valuable fuels. Developing efficient and selective electrocatalysts is a key requirement for these processes. In this approach, the Ag-Cu electrode is prepared by electrodeposition. The electrodeposition process can be optimized to control the surface morphology and composition of the Ag-Cu electrode, which can impact its catalytic performance for CO_2 reduction. CO_2 reduction products were quantified by nuclear magnetic resonance spectroscopy and gas chromatography.

Poster Presentation : **ENVR.P-460**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Variation of CO2RR product distribution according to P and S composition of Cu based catalyst

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Electrochemical CO2 reduction reaction(CO2RR) is drawing attention since it can replace fossil fuels and convert CO2 into valuable carbon compounds by using electricity generated from renewable energy. Among many materials active in CO2RR, Copper(Cu) has an appropriate value for adsorption energy of CO2 as a reactant and desorption energy of *CO as an intermediate. Therefore, Cu-based catalysts are receiving a lot of attention because they are advantageous for producing multi-carbon compounds. It is known that one of them, a CuS-type catalyst and a CuP-type catalyst, show different product distributions. Several studies have reported that this is because the degree of adsorption of the reactant CO2 and its intermediates on the catalyst surface is different. Based on these previous research results, We newly synthesized Cu-P-S type catalysts with various composition ratios and proceeded with basic characterization of the catalysts. In addition, the activity of CO2RR was tested and the change in product distribution and its cause were identified

Poster Presentation : **ENVR.P-461**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Controlling the Rates of the Degradation of the Mulch Films

Yeonkyeong Ryu, Kyung-An Kim, Hyun Gil Cha[1,*]

Center for Bio-based Chemistry, Korea Research Institute of Chemical Technology, Korea
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The degradable mulch films are widely used in the agriculture increasing the yield of crops with constant humidity and nutritious content of the soil. Chemical additives and composites are suggested to control the rate of degradation of the mulch film polymers. Various mechanistic routes are proposed to accelerate and decelerate the depolymerization/degradation.KeywordsMulch film, Degradable polymers, Polymer degradation, Polymer additivesAcknowledgementsThe Cooperative Research Program for Agriculture Science and Technology Development (PJ01708204) through the Rural Development Administration and the core project (KS2342-10) from Korea Research Institute of Chemical Technology (KRICT) are acknowledged for support.

Poster Presentation : **ENVR.P-462**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photocatalytic degradation of Bisphenols over K and Na-loaded Titanium oxide based nanostructures

Juyoung Maeng, Kim So Young, Jeongkwon Kim[1], Choong Kyun Rhee[1], Youngku Sohn[1,*]

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

This study investigates the photocatalytic degradation of bisphenol using a TiO_2-based catalyst. The catalyst was prepared through hydrothermal synthesis, in which K and Na were loaded onto the surface of TiO_2 to grow nanostructures. The effectiveness of the catalyst was evaluated by decomposing various bisphenols under UVC irradiation, and the resulting degradation products were analyzed using liquid chromatography mass spectrometry. Additionally, density functional theory calculations were employed to obtain information on electronic energy levels and chemical bond energies. The results demonstrate that the TiO_2-based catalyst is highly effective in the photocatalytic degradation of bisphenol.

Poster Presentation : **ENVR.P-463**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Photocatalytic degradation of bisphenols and photoluminescence properties of Eu (III)-doped $CaTiO_3$, $BaTiO_3$ and $SrTiO_3$ nanoparticles

Soyoung Kim, Juyoung Maeng, Goeun Park, Seo Young Yang, Seon Young Hwang, Jeongkwon Kim[1], Choong Kyun Rhee[1], Youngku Sohn[1,*]

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

In this work, Eu (Ⅲ)-doped perovskite $CaTiO_3$, $BaTiO_3$ and $SrTiO_3$ nanoparticles (NPs) were synthesized by solvent evaporation followed by thermal treatment. A photoluminescence study showed that the $CaTiO_3$ support showed the highest red emission intensity, attributable to the transition of Eu (III) ion. Photocatalytic CO_2 reduction was observed to produce mainly CO and CH_4 under UVB, UVC. The efficient catalysts according to each UVB and UVC were $SrTiO_3$ and $BaTiO_3$ nanoparticles. Photocatalytic degradation and the corresponding kinetics of bisphenol AF and bisphenol S have been presented in this present work and a simple mechanisms have also been explored.

Poster Presentation : **ENVR.P-464**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrocatalytic CO_2 reduction of In and In alloys for electrochemical and surface compositions

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[1]Chungnam National University, Korea
[2]Chemistry, Chungnam National University, Korea

Indium in the p-block is known for its high Faradaic efficiency in electrochemically reducing CO_2 to formic acid. To investigate the products formed under different voltages and the changes in the electrode surface and composition, experiments were conducted using In electrodes and In alloys such as InBiSn and InSn electrodes. The results showed that the InSn electrode had the highest efficiency, with a Faradaic efficiency of 96.82 % under the $KHCO_3$ electrolyte condition. Bare In electrodes showed a FE of 90.2% and for formate production at -1.8 V (vs. Ag/AgCl) under 0.1 M $KHCO_3$ condition. And InSn electrode show the highest FE of 97.7% in 0.2 M $KHCO_3$ electrolyte. The chemical state of the electrode surface was also analyzed using X-ray photoelectron spectroscopy after the CO_2 reduction reaction.

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April 26(Wed)~28(Fri), 2023, Suwon Convention Center, Korea

Poster Presentation : **ENVR.P-465**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrocatalytic CO_2 reduction over Annealed Cu-Sn alloy electrode

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Electrochemical CO_2 reduction (CO_2RR) is a promising technology for producing valuable products from CO_2. In this study, we investigated the production of highly selective ethylene and methane using an annealed Cu-based alloy. Gas chromatography and NMR spectroscopy were utilized to identify the products of CO_2 reduction, which confirmed the formation of CO, CH_4, $HCOO^-$, $CHCOO^-$, and CH_3OH. The electrode surface morphology and elemental oxidation states were analyzed using scanning electron microscopy and X-ray photoelectron spectroscopy, respectively. The results obtained from the annealed Cu-based alloy demonstrate high Faradaic efficiency and selectivity, which provides valuable information for practical CO_2 recycling.

Poster Presentation : **ENVR.P-466**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrochemical CO_2 reduction over thermal-treated Ag/Brass electrode

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Scientists are exploring CO_2 recycling as a solution to the concerns around increased CO_2 concentration and fossil fuel shortages. This study introduces a thermal-treated Ag/Brass electrode for electrochemical CO_2 reduction, which produced various gas and liquid products. The study found that the Faradaic efficiencies of the products were dependent on experimental conditions, and that the introduction of thermal-treated Brass with Ag dramatically increased the FE of CH_4. Surface elemental oxidation states were examined using X-ray photoelectron spectroscopy, providing useful information for the production of CH_4 from CO_2 through electrochemical CO_2 reduction. This has important implications for energy and the environment.

Poster Presentation : **ENVR.P-467**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Galvanic Substitution of Ag in Cu-Mesh Electrodes for Enhanced Electrochemical CO_2 - to - CO Conversion

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Electrochemical CO_2 reduction using Copper (Cu) electrodes can produce various products such as CH_4 and C2 compounds. In this study, we aimed to induce the production of CO through galvanic substitution of Silver (Ag) in Cu-mesh. We compared the effect of varying the galvanic substitution time to observe the thickness of the substituted Ag. The electrochemical CO_2 reduction products were analyzed using gas chromatography and nuclear magnetic resonance spectroscopy. Additionally, we examined the fundamental properties of the electrode using scanning electron microscopy, X-ray photoelectron spectroscopy, and energy dispersive X-ray spectroscopy. We observed that the Faradaic efficiency of CO increased as the thickness of the substituted Ag increased. We also discussed the relationship between the Faradaic efficiency and the nature of the developed electrode.

Poster Presentation : **ENVR.P-468**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Electrochemical reduction of CO_2 using Ag, Au, and Cu/bronze electrocatalysts

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Bronze is recognized for its high electrochemical efficiency and selectivity in reducing CO_2. In this study, we loaded bronze electrodes with Ag, Au, and Cu metals and tested their electrochemical CO_2 reduction properties. Gas chromatography and nuclear magnetic resonance spectroscopy confirmed that the major reduction products were CO, CH_4, ethanol, and formate. Faraday efficiency was used as a measure of selectivity. The oxidation states of the electrodes were evaluated using X-ray photoelectron spectroscopy and scanning electron microscopy before and after CO_2 reduction.

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Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Investigation on synthesis and properties of isosorbide diglycidyl ether as secondary building block

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Isosorbide (ISB) is a representative compound as an advantageous competitor of petroleum-derived components in the synthesis of polymers of different nature. When the reactivity of isosorbide is not enough, it can be successfully transformed into secondary building blocks, such as isosorbide diglycidyl ether, which provides extra functionalities for the synthesis of polyurethanes/epoxy resin. In this study, the physicochemical properties of each isosorbide diglycidyl ether were compared to create an adaptation route of the synthetic method for application to polymers.Keyword//Isosorbide; Isosorbide diglyceryl ether; Physicochemical properties; Adaptation route; Synthetic method. AcknowledgementsThis work was supported by Korea Environment Industry & Technology Institute(KEITI) through Technology Development Project for Safety Management of Household Chemical Products Program, funded by Korea Ministry of Environment(MOE) (RE202201835) and Korea Research Institute of Chemical Technology (KRICT) core project (KS2342-10).

Poster Presentation : **ENVR.P-470**
Environmental Energy
Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Lifetime Prediction of Li-ion Pouch Batteries with Machine Learning-based Method

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As society's use of fossil fuels has led to environmental pollution and a climate crisis, there is a growing focus on alternative energy sources that are more environmentally friendly. Electric vehicles are gaining attention as a promising method of transportation for the future. The key technology behind electric vehicles is the lithium-ion battery and its battery management system (BMS). However, measuring and improving the performance of these batteries over time can be a time-consuming process due to their long lifespan. Additionally, it is challenging to accurately measure the state of charge (SOC) and state of health (SOH) of the batteries in real-time due to the many variables that affect their operation. Fortunately, advances in machine learning have enabled accurate predictions to be made without relying on complex physical knowledge, using high-quality data instead. In this study, we used machine learning technology to analyze the charge/discharge data of lithium-ion batteries. We selected the measured values from the initial charge/discharge cycles as the independent variable and the number of cycles remaining until the battery's end of life as the dependent variable. A recursive neural network (RNN) was applied to the data, followed by model tuning to increase accuracy and reduce overfitting. Through this approach, the researchers were able to accurately predict the state of health (SOH) of a lithium-ion battery using only the initial cycles, which contributes to real-time data collection for battery management systems (BMS) and improves the efficiency of the study.

Poster Presentation : **ENVR.P-471**

Environmental Energy

Exhibition Hall 2+3 (1F) FRI 11:00~13:00

Spectroscopic studies of aggregation-induced emission (AIE)-based plastics dye.

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A novel pyrene-based fluorescent dye L was developed for investigating spectroscopic characteristics. It exhibited a green fluorescence enhancement as the amount of water increased. A tyndall phenomenon of L supported its novel characteristic of AIE. A solvatochromic study of L exhibited bathochromic shifts on increasing solvent polarity. Based on the solvatochromic study, L showed the most prominent AIE properties in the THF/DIW mixture (1:9, v/v). This study was supported by the Human Resource Development Programs for Green Convergence Technology funded by the Korea Ministry of Environment (MOE).